Computational Intelligence Techniques for Decision Making

with Applications to the Dairy Industry

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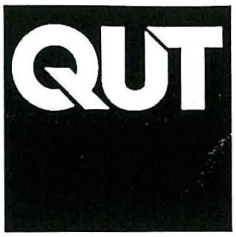

QUEENSLAND UNIVERSITY OF TECHNOLOGY

DOCTOR OF PHILOSOPHY THESIS EXAMINATION

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Under the requirements of PhD regulation 16.8, the above candidate presented a Final Seminar that was open to the public. A Faculty Panel of three academics attended and reported on the readiness of the thesis for external examination. The members of the panel recommended that the thesis be forwarded to the appointed Committee for examination.

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FORM B

Keywords

allocation, ant colony optimisation, classification, constraint logic programming, dairy, decision trees, differential evolution, genetic algorithms, heuristics, immune systems, intelligent decision support systems, knowledge discovery in databases, mate-selection, neural networks, optimisation, prediction, simulated annealing, tabu search

Abstract

The dairy industry is a major resource in the Australian economy. In 1995-96 there were 13,888 dairy farms[1] in Australia with 1.924 million dairy cows [2] and a total milk production of 8,716 million litres with a combined value of $AUD3 billion on the wholesale level. The industry's success is dependent on increased animal productivity through breeding programs and efficient management. One of the main challenges in the industry therefore, is to improve the productivity of breeds through the design of efficient breeding programs. These programs aim to improve the genetic merit as well as the productivity of animals through identifying (*selecting*) and mating (*allocating*) animals with high genetic values, under the prevailing environmental and managerial conditions. To solve the selection and allocation problems, we need to predict the progeny's expected productivity (*ie.* milk, fat, and protein yields) arising from any mating.

From the previous discussion, the task of building a breeding program can be decomposed into three interrelated stages: prediction, selection, and allocation. In prediction, the expected merit of potential progeny is estimated from information collected and recorded about their parents and the environment. In selection, a set of sires and a set of dams are chosen for mating according to the overall goal of the program. In allocation, individual matings among the selected animals are decided according to the expected progeny merit as well as some preferences and goals. Reaching an optimal decision is only possible when both selection and allocation are solved simultaneously and in this case the problem is called *mate-selection.* The problem is hard when the planning is for a single generation to optimise a short-term goal. In long-term planning, additional objectives need to be considered such as the minimisation of inbreeding (*ie.* matings of related individuals). As a result, nonlinearity and conflicting objectives arise within the problem. Mate-selection decisions require progeny prediction and other information that can be retrieved from the databases currently kept by the farmers and their organisations for production and pedigree records.

The objective of this thesis is to integrate *Knowledge Discovery from Databases* (KDD) with the *Intelligent Decision Support System* (IDSS) paradigm, to comprise what we call in this thesis

[1]Source: Australian Dairy Corporation ADC.

[2]Source: Australia Bureau of Statistics.

KDD-IDSS, for designing efficient breeding programs. To achieve this objective, we define three sub-objectives: (1) to design a generic kernel for the KDD-IDSS. (2) to discover patterns in the dairy database using KDD, and (3) to formulate and solve one version of the mate-selection problem. The first objective is achieved by designing a novel constraint logic programming based language to abstract general operational research and artificial intelligence modules within the KDD-IDSS. The second objective of the thesis is accomplished in two steps; first, by discovering effective predictive patterns to update the predictive model in the model base of the IDSS. Second, by generating a knowledge base to describe the reasoning behind a certain mating using a comparison between a rule extraction technique, RULEX, and a decision tree classifier, C5, to update the knowledge base of the KDD-IDSS. This required the use of a bayesian clustering method, Autoclass, for grouping the cows according to their milk production. This second objective of the thesis evolved a new method, C-Net, for generating dynamic and non-deterministic decision trees. The method achieved a balance between the predictive accuracy of neural networks and the language expressiveness of decision trees.

The third objective is attained through a formulation of a general optimisation model for mate-selection. A number of existing heuristic techniques (ant colony optimisation, genetic algorithms, immune systems, and simulated annealing), and three newly developed ones (Markov chain Tabu search, evolving colonies of ants, and dynamic adjustment method), are compared for solving this model. The two most successful models were Markov chain Tabu search and evolving colonies of ants. Both models were significantly better than the other heuristics. The overall objective of the model is to issue the farmer with a mating plan for one-generation resulting from the optimal strategy for a number of generations.

Overall, the three objectives will make a solid ground for building successful breeding programs that the industry can use. In so doing, the expected profitability of the dairy industry will increase on the long term and the current softwares for solving our proposed mate-selection problem will be able to handle larger problem sizes.

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- Journals

  - H.A. Abbass, M. Towsey, and G.D. Finn. "C-Net: A method for generating non-deterministic and dynamic multivariate decision trees". *International Journal of Knowledge And Information Systems (KAIS)*, Springer Verlag, accepted for a forthcoming issue.
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List of Acronyms

ABV	Australian Breeding Value
ACO	Ant Colony Optimisation
AI	Artificial Intelligence
AI-sire	Artificial Insemination sire
ANN	Artificial Neural Networks
BP	Back-Propagation
BV	Breeding Value
CLP	Constraint Logic Programming
DE	Differential Evolution
DT	Decision Tree
EBV	Estimated Breeding Value
FLMV	First Lactation Milk Volume
GA	Genetic Algorithms
IDSS	Intelligent Decision Support systems
KDD	Knowledge Discovery in Databases
LMV	Lactation Milk Volume
LRU	Local Response Unit
MCTS	Markov Chain Tabu Search
MDT	Multivariate Decision Tree
MLP	Multi-Layer Perceptron
MLR	Multiple Linear Regression
MSI	Mate-Selection Index
MV	Milk Volume
NT	Number of traits
OR	Operations Research
PTL	Probabilistic Tabu List
PTS	Probabilistic Tabu Search
RDT	Recurrent Decision Tree
RMSE	Root Mean Square Error
SA	Simulated Annealing
SI	Selection Index
SLMV	Second Lactation Milk Volume
TS	Tabu Search
UDT	Univariate Decision Tree
VOP	Vector Optimisation Problems

Table 1: List of Acronyms used throughout the thesis

List of Mathematical Abbreviations

$(\ )^t$	is the transpose of a vector. Unless indicated otherwise, the default is a column vector.
S.T.	Subject to
Φ	Empty set
$\in$	Belong to
$\ni$	Such that
$\mid$	Given
$\rightarrow$	Maps to
$\exists$	There exists
$\nexists$	There exists no
$\forall$	For all
$\cap$	Intersection
iff	If and only if
$\ncong$	Not equal to for vectors
$\precsim$	Less than or equal to for vectors

Table 2: List of mathematical abbreviations used throughout the thesis

Statement of Original Authorship

The work contained in this thesis has not been previously submitted for a degree or diploma at any other higher education institution. To the best of my knowledge and belief, the thesis contains no materials previously published or written by another person except where due reference is made.

Date: 16/3/2001

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Part I

Introduction

Chapter 1

Thesis Outlines and Contributions

The process of creating a breeding system for the Australian dairy industry's artificial insemination program naturally divides into a prediction problem and an optimisation problem. In the former, the objective is to predict the performance of offspring based on some of the genetic traits of their parents. In the latter, two component sub-problems can be identified, selection and allocation. In selection, a set of sires and a set of dams are selected for possible mating based on some suitable criteria for improving animal traits; in allocation, specific matings are allocated among the selected animals. Solving both problems independently does not guarantee an optimal solution overall. To achieve an optimal solution, a mathematical model that selects and allocates simultaneously, called *mate-selection*, is required.

The objective of this thesis is to develop appropriate problem solving techniques for the efficient design of dairy cattle breeding systems through the integration of *Knowledge Discovery from Databases* (KDD) with the *Intelligent Decision Support System* (IDSS) paradigm, to comprise what is called *KDD-IDSS*. This objective is decomposed into three sub-objectives:

1. designing a generic kernel (*ie.* an interface language between the system's components) for the KDD-IDSS,
2. discovering patterns in the dairy database using KDD, and
3. formulating and solving a mate-selection problem.

The thesis begins with a description of the general mate-selection problem. An information system framework is then developed for this problem. The framework is based on the integration of

KDD and IDSS. A proposed generic meta-language for an interface component of the framework is then introduced using the constraint logic programming paradigm.

The prediction problem is then investigated in two stages. The first stage is concerned with point-estimation where a linear regression model is compared against a feed-forward neural network. The second stage is concerned with extracting symbolic knowledge from the database and is handled by a comparison between a rule-extraction technique, RULEX, and a decision tree classifier, C5. The powers of neural network and decision trees are then combined into a novel algorithm for generating dynamic and non-deterministic decision trees. Following this, a version of the mate-selection problem is formulated and problem-solving approaches are developed. Below, the detailed thesis outlines are presented.

1.1 Thesis outlines

The thesis is divided into eleven chapters as described below:

In Chapter 1, an introduction to the thesis is presented, followed by the thesis outlines and a list of scientific contributions.

The main objective of Chapter 2 is to provide the basic concepts of the domain of application, necessary to build upon the case study of mate-selection pursued in this thesis. The chapter starts with an introduction to Genetics in Section 2.1, followed by a review of the basic animal breeding concepts in Section 2.2. Two problems are then identified: *selection* and *allocation*. In Section 2.3, different methods for selection of animals for breeding are discussed, then different recent strategies for selection are elucidated in Section 2.4. Methods for allocation of animals for mating are followed in Section 2.5. A review of some computer programs for selection, is then presented in Section 2.6. Conclusions are drawn in Section 2.7.

The *information system framework* for the thesis is then introduced in Chapter 3, beginning with a decision making process summary in Section 3.1, followed by a literature review of *intelligent*

decision support systems (IDSSs) in Section 3.2 and *knowledge discovery in databases* (KDD) in Section 3.3. The proposed framework for integrating KDD with IDSS, called KDD-IDSS, is then presented in Section 3.4. A proposed meta-language is then designed using *constraint logic programming* (CLP) for integrating *operations research* (OR) and *artificial intelligence* (AI) components in the KDD-IDSS frame. The three dimensions for the integration are covered in Section 3.5; these are integrating CLP with optimisation, CLP with AI, and optimisation with AI. The language is then formulated in Section 3.6 followed by an example of the usefulness of this formulation in Section 3.7. Conclusions are drawn in Section 3.8.

In Chapter 4, the experiments carried out for the data mining component are presented. Experimental design and objectives are presented in Section 4.1 followed by a review of the mining techniques that will be used in the chapter starting with an introduction to multi-layer feed-forward *artificial neural networks* (ANNs) in Section 4.2 followed by *Bayesian clustering* in Section 4.3 and *classification decision trees* (DTs) in Section 4.4. A description of the database is then presented in Section 4.5. Following this, two experiments are discussed: point estimation in Section 4.6 and interval estimation in Section 4.7. The first experiment's objectives are to investigate their predictive power on the progeny performance and to identify a prediction model that can be used in the KDD-IDSS's model base. The second experiment is concerned with the automatic extraction of symbolic knowledge to reason about the choice of a mating. This is similar to the point-estimation's experiment, except for the necessity of discretising the output where Autoclass, a Bayesian clustering algorithm, is used for this purpose. Conclusions are drawn in Section 4.8.

The experiments, presented in Chapter 4, motivated a novel algorithm, C-Net, used for integrating ANNs and DTs. This algorithm is the focus of Chapter 5. The importance and motivation of this algorithm are introduced in Section 5.1 followed by previous work in combining ANNs and DTs in Section 5.2 and the C-Net algorithm in Section 5.3. In Section 5.4, experimental results and comparisons are discussed and the dynamic version of C-Net is then scrutinised in Section 5.5. Conclusions are drawn in Section 5.6.

In Chapter 6, the foundation of the heuristic techniques that will be used for solving the mate-

selection problem's version that is being addressed in this thesis, are presented. The chapter begins with an introduction to optimisation theory in Section 6.1. Seven heuristic search techniques are then presented, more specifically; *simulated annealing* (SA) is presented in Section 6.2 followed by *tabu search* (TS) in Section 6.3, *genetic algorithm* (GA) in Section 6.4, *differential evolution* (DE) in Section 6.5, *immune systems* (Immune) in Section 6.6, *ant colonies optimisation* (ACO) in Section 6.7, and *memetic algorithms* (MA) in Section 6.8. Issues arising from constraints and multi-objectives are discussed in Sections 6.9 and 6.10, respectively. Conclusions are drawn in Section 6.11.

In Chapter 7, our proposed version of the mate-selection problem is formulated as a multi-stage optimisation model. An introduction about allocation is presented in Section 7.1, followed by the importance of mate-selection in Section 7.2. In Section 7.3, the problem is formulated, and the complexity of its search-space is discussed in Section 7.4. Conclusions are drawn in Section 7.5.

In Chapter 8, the single-stage mate-selection problem is derived from the generic formulation and a set of GA operators that results in a good solution of the single-stage model, is identified. In Section 8.1, a case study is presented with ten herds where cows were mated solely to artificial insemination bulls. In Section 8.2, a genetic algorithm design for the single-stage model is presented followed by a number of experiments with the aim of identifying a set of genetic algorithm operators that reach the optimal solution quickly and reliably in Section 8.3. Conclusions are drawn in Section 8.4.

In Chapter 9, the multi-stages mate-selection problem is derived from the generic formulation and different heuristics are applied to solve the model. In Section 9.1, the derivation of the model is shown, followed by the experimental design in Section 9.2. Different strategies for solving the model are then presented in Sections 9.4, 9.5, 9.6, 9.7, 9.8, 9.9, 9.10, 9.11, and 9.12. Lastly, Section 9.13 presents an overall comparison between the proposed solution strategies. Conclusions are drawn in Section 9.14.

In Chapter 10, the proof for the existence and non-uniqueness of the mate-selection index is established in Section 10.2. Two methods for generating this index are then introduced in Sec-

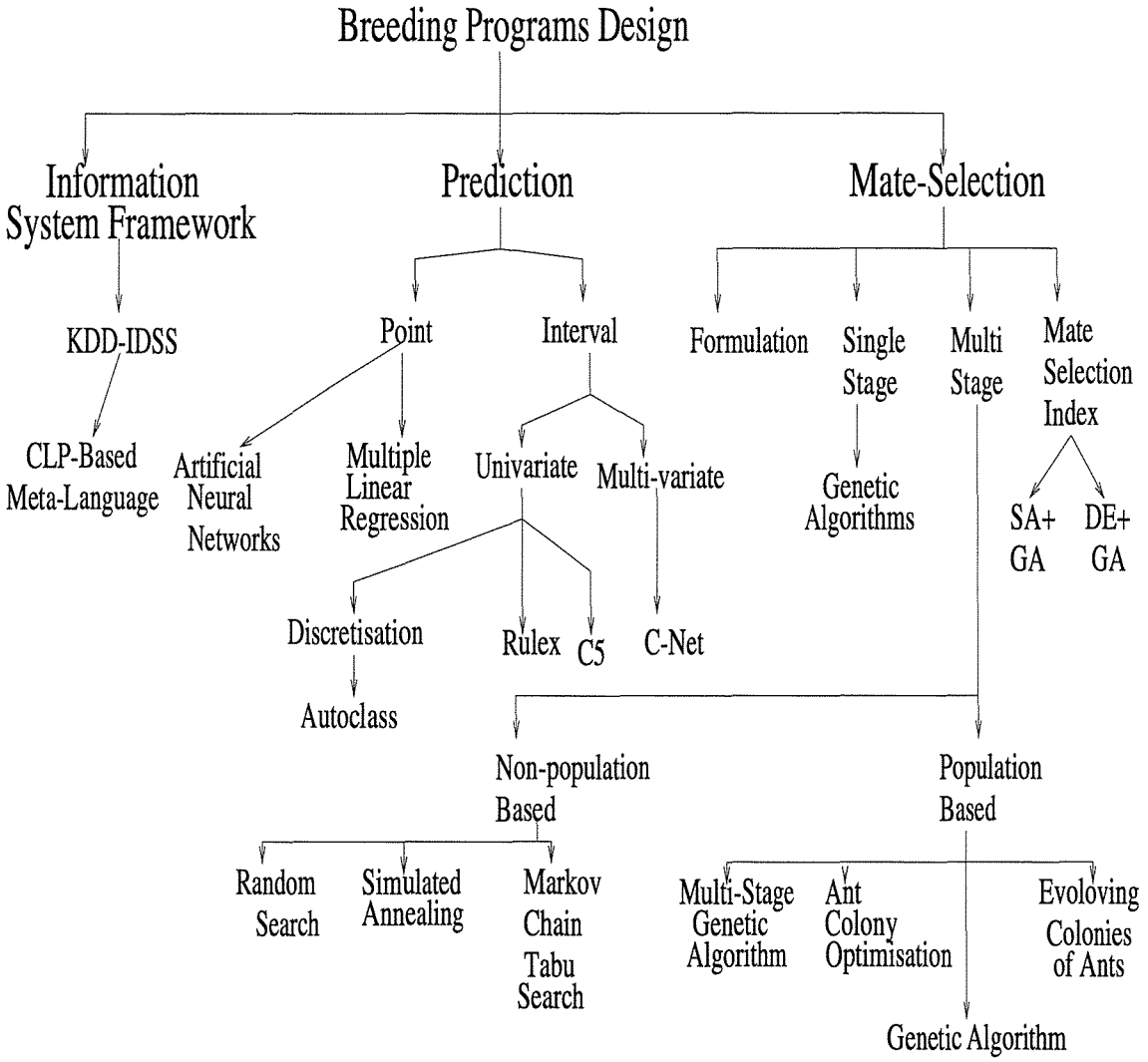

Figure 1.1: A conceptual tree of issues and techniques discussed in this thesis.

tions 10.3 and 10.4. Conclusions are drawn in Section 10.5.

In Chapter 11, conclusions about the thesis findings are drawn and points for further research are discussed. This chapter concludes the thesis.

A conceptual diagram representing different techniques in the thesis and the overall structure is given in Figure 1.1.

1.2 Original contributions

The following original contributions have been achieved in this thesis and are listed below:

1. In Chapter 3, a new generic frame, KDD-IDSS, for integrating knowledge discovery in databases with intelligent decision support systems is proposed.

2. Chapter 3 also proposes a constrained logic programming based meta-language for interfacing OR and AI models in the KDD-IDSS frame.

3. In Chapter 4, the knowledge governing the outcome of a mating is extracted from the dairy database.

4. Chapter 5 presents a novel algorithm, C-Net, for generating non-deterministic and dynamic decision trees.

5. Chapter 7 introduces a generic formulation for our proposed mate-selection problem, and to my knowledge, is a first time attempt to study the overall problem's complexity.

6. In Chapter 8, the single-stage mate-selection model is derived from the generic formulation as a quadratic transportation model, and genetic algorithm is used to solve the model. A new crossover operator, gene-based crossover, and a repair operator are developed.

7. In Chapter 9, a proposed mate-selection problem for farms depending on artificial insemination is derived from the generic model. Two novel algorithms, Markov chain Tabu search, and evolving colonies of ants, are developed.

8. In Chapter 10, a new method for creating a mate-selection index, called dynamic adjustment of the objective function, is introduced. The existence and non-uniqueness of the mate-selection index is proved mathematically.

Chapter 2

Mate-Selection in Animal Breeding

Designing a breeding program is one of the issues that animal breeding research has focused on, in recent decades. Generally the outcome of a breeding program is a long-term product and requires careful design. Two crucial components in a breeding program are the definition of a suitable breeding objective(s) and the *mate-selection* problem. The latter is in two parts: first, *selection* or which animals will be selected for mating and which for culling; and second, *allocation* or the choice of the suitable mating pairs among those animals selected for mating.

In this chapter, the mate-selection problem is scrutinised. The genetic background necessary to introduce it, is presented in Section 2.1 followed by basic concepts in animal breeding in Section 2.2. Section 2.3 introduces different methods for selection of animals for breeding, and different recent strategies for selection are then elucidated in Section 2.4. Methods for mate-selection follow in Section 2.5, concluded with a review of some computer programs for selection in Section 2.6. This chapter's main objective is to provide the basic concepts of mate-selection necessary to build upon the case study pursued in this thesis.

2.1 Genetics

The word *genetics* derives from the Greek root $\gamma\epsilon\nu\nu\omega$, which means "to become" or "to grow" (Winchester 1966). The classical definition of genetics introduced by William Bateson, who named the field of study in 1906 (Schmidt and Van-Vleck 1974), is:

> genetics is the science dealing with heredity and variation seeking to discover laws

governing similarities and differences in individuals related by descent (Van-Vleck et al. 1987).

In short, genetics is the science of inheritance (Daniel 1994). The *gene* is a chemical entity that influences an inherited trait from parents to their children. Each gene, at a given *locus*, can take various forms called *alleles*. For example, if the colour of an animal is either white, black, or gray, it is determined according to a pair of genes with the alleles "w" for white and "b" for black. If the pair of genes is the same (eg. "ww" for a white animal or "bb" for a black one), the organism is called *homozygous* otherwise *heterozygous* (eg. "wb" for a gray animal). If the animal is heterozygous and an allele conceals the effect of its pair member (*eg.* the pair of genes is "wb" and the colour is black), it is called *dominant*, "b", otherwise *recessive*. A group of chromosomes constitutes the organism's *genotype* which is the genetic constitution or sometimes called the genetic makeup (Falconer 1989). The observable traits of an organism constitute its *phenotype* (Daniel 1994).

The science of genetics was discovered by the Austrian monk Gregor Mendel in 1865 (Franisco and John 1984). Mendel introduced two laws that were rediscovered in 1900 by the European botanists Correns, De-Vries, and Tschermark. The first is the law of *"segregation"* which defines the amount of genetic materials transmitted during a mating. It states that during combination, a gene pair separates into the reproductive or sex cells formed by an individual, so that half carry one member of the gene pair and half carry the other (Van-Vleck et al. 1987). The second is the law of *"independent assortment"* which states that "*during gamete formation, segregating pairs of unit factors assort independently of each other*" (Klug and Cummings 1999). *Unit factors* (Klug and Cummings 1999) are particulate for each trait which serve as the main units of heredity and are passed unchanged from generation to generation, determining various traits expressed by each individual. From these two laws we can define what is called a *Mendelian sampling.* Since the segregation of genes occurs independently, and half of the gene pair is transmitted to the offspring during the mating, there is no guarantee which gene will be transmitted. Accordingly, although we know that the progeny have one half of their father's and their mother's genes, siblings will differ since they will take different combination of genes. The variation due to this sampling causes variation within full sib families, and is indicated as the Mendelian sampling. A formal equation for it will be defined later in this chapter.

In 1908, British mathematician G.H. Hardy and German physician W. Weinberg introduced the *Hardy-Weinberg equilibrium law* (Franisco and John 1984), forming the basis of population genetics. The law assumes an absence of selection and states that the process of heredity changes neither allelic frequencies nor genotypic frequencies at a given locus within a very large, closed, randomly breeding population. Additionally, the *equilibrium genotypic frequencies* at any given locus are attained in one single generation of random mating whenever the allelic frequencies are the same in the two sexes.

Mendelian genetics studies the principles of transmitting the genetic material from the parents to the offspring generation. *Population genetics* is the study of Mendelian genetics in populations. It is concerned with the frequencies of genotypes and phenotypes (Falconer 1989), and is limited to the inheritance of qualitative traits. *Quantitative genetics* was introduced by Fisher in 1918 and is concerned with the study of the effects of individual genes (Van-Vleck et al. 1987), as well as the study of correlation and regression between the genetic and phenotypic values. As opposed to population genetics, it concentrates on quantitative traits.

The *qualitative traits* (Daniel 1994) are those traits controlled by one or a few loci, in a way that allele has a marked effect on the phenotype and individuals can be phenotypically classified into one of a group. For example, the human blood groups designated A, B, O, or AB are determined by three types of alleles denoted IA, IB, and IO. The blood group of any person is determined by the particular pair of alleles present in his or her genotype. In *quantitative traits*, there are many loci, a gradation of phenotypes, and small effects of single alleles. Quantitative traits usually follow a normal distribution (Falconer 1989) and can be found in three categories, *continuous*, *meristic* and *threshold* traits (Franisco and John 1984). Continuous traits vary, with no clear-cut breaks, from one phenotypic extreme to the other, such as milk production in cattle. In Meristic traits, the phenotype is determined by such counting as the number of eggs laid by a hen. Threshold traits have only two or few phenotypic classes, but their inheritance is determined by the effects of multiple genes together with the environment, such as twining in cattle.

The phenotypic value of an animal trait (Schmidt and Van-Vleck 1974) is measured by the difference between the animal's trait value and an appropriate base group. This base group can be the average of all animals within the herd born in the same year, the herd average at the breeding program's commencement, or any other appropriate base. The phenotypic value (P) (Schmidt and Van-Vleck 1974) of an animal for a specific trait is the sum of the animal genotypic value (G) and the environmental deviation (E); that is

$$P = G + E \tag{2.1}$$

The environmental deviation is a term used in the field to represent the effects of all non-genetic factors such as seasons, feeding systems, management, etc. An animal's genotypic value can be further decomposed into three measurements: the breeding or the additive genetic value (A), the dominance deviation (D), and the epistasis or interaction deviation (I).

$$G = A + D + I \tag{2.2}$$

Gene action is said to be additive if the differences between the heterozygote and the two homozygotes are equal (Schmidt and Van-Vleck 1974). Inheritance depends on the additive effects of genes and represents the value of an individual's genes to its progeny. Generally, the offspring inherit only the average additive component of their parents. The dominance deviation causes a heterozygous animal to be more like one of the homozygous genotypes. For example, assume a homozygous black cow is worth \$4 and a homozygous red cow is worth \$2. If the gene for black colour is dominant, a heterozygous cow will look black and will be worth \$4 although it should be worth only \$3 ($\frac{4+2}{2}$). The \$3 represents the additive genetic value and the additional \$1 represents the dominance deviation. The epistasis is a measure of the effect of other genes on the gene in question; that is, sometimes the expression of an allele at a locus requires the presence of a particular allele at another locus. Now, we can rewrite the equation for the phenotypic value as:

$$P = A + D + I + E \tag{2.3}$$

A basic concept in genetics is *heritability.* To illustrate this concept, the concepts of phenotypic and genotypic variances are presented. The phenotypic variance, V_P, is the sum of the population genotypic variance, V_G, and the environmental variance, V_E; that is

$$V_P = V_G + V_E \tag{2.4}$$

where

$$V_G = V_A + V_D + V_I \tag{2.5}$$

and V_A is the additive genetic variance whereas the sum of V_D and V_I is the non-additive genetic variance (dominance and epistasis). Heritability, h^2, is the ratio between the additive genetic and phenotypic variances; that is

$$h^2 = \frac{V_A}{V_P} \tag{2.6}$$

Since V_A is always less than V_P, the heritability is always in the range [0,1]. The higher the heritability, the more important it is for the breeder to use breeding systems which utilise the additive genetic variation. One way; although not necessary the best, to estimate the heritability of a trait is to regress the offspring on the parents; that is, the correlation coefficient between the offspring and the parents phenotypic values for the trait. However, it is better to use multi–trait animal models because they use all the available information from relatives.

Animal genetics is the study of the principles of inheritance in animals whereas animal breeding applies these principles with the goal of animal improvement (Van-Vleck et al. 1987). This study will be concerned with quantitative genetics, especially the continuous traits, for dairy cattle.

2.2 Breeding programs

Cattle are a *monotocous* species; the female produces a single egg at a time and consequently normally produces a single offspring each parity. They form one of the main agricultural resources in Australia. In 1995-96, there were 13,888 dairy farms[1] in Australia with 1.924 million dairy cows [2] and a total milk production of 8,716 million litres with a value of $3 billion on the wholesale level. The industry success depends on increased animal productivity through breeding programs and efficient management.

A breeding program's main objective is to maximise the progeny's productivity measured with their *production traits*. The merit of breeding animals is estimated using the *(estimated) breeding*

[1]Source: Australian Dairy Corporation ADC.

[2]Source: Australia Bureau of Statistics.

values (EBVs) which define the (estimated) value of an animal in a breeding program, measured in terms of the expected progeny performance relative to the population mean. The breeding value is twice the difference between the expected offspring mean and the mean population (genotypic) value. The breeding value is referred to as the animal's *additive genetic merit.* (Van-Vleck et al. 1987)

The breeder requires a system to screen the genotypes to select the animals with the highest breeding value (the measures computed by screening programs are used for selecting bulls and cows for mating). An animal's merit in a selection decision depends on both the value of future progeny (genetic value) and their own expected performance (production value). The process of selecting animals as future parents in the herd uses either a *selection index* (for long term planning) or *production index* (for short term planning) (Garner et al. 1995). The former expresses the likely merit of an animal's progeny, thereby indicating its worth as a breeding animal. A set of *economic weights* is employed to express economic preferences among different traits. For the latter, the economic weights in the selection index are replaced by the actual profit represented by a profit function. Furthermore, if the breeding program is designed for the short term, selection should be based on the real producing ability (*ie.* a percentage of the difference between the animal production record and the herd average (Schmidt and Van-Vleck 1974)). If the program is designed for the long term, selection should be based on the genetic gain. In practice, a combination of both short and long term objectives is required.

Two potential sources of information exist that may determine the breeding value of animals - the pedigree and performance data. The *progeny deviation* represents the parents' transmitting ability. Accordingly, a *progeny test* is undertaken by mating an animal to obtain progeny for observation. The probability that the estimated breeding value is a good estimate of the true breeding values increases with the number of progeny records available for each animal. This introduces the *reliability* of a breeding value, which equals the square of the correlation between true and estimated breeding values. In the *Australian breeding values* (ABVs), a sire ABV is qualified for publication if it has at least 15 effective (productive) daughters across 5 herds (ADHIS 1997). Generally, if a cow has one performance record, the reliability of her milk figure is 25%, which is the heritability of milk (Schmidt and Van-Vleck 1974). Six records about the

cow with 50 paternal half sisters is enough to reach 70% reliability (Van-Vleck et al. 1987). The breeder's computer system is used to provide information that assists in measuring the two crucial parameters in any breeding program - genetic gain and inbreeding.

Genetic Gain

One of the key objectives of breeding program design is to maximise herd's genetic improvement or gain. There are four main factors that control genetic improvement (Schmidt and Van-Vleck 1974): variation, intensity of selection, accuracy of selection, and generation interval. The genetic gain per year, assuming a large population as the normal case in practice, is generally measured by the following equation:

$$Genetic\,gain/year = \frac{\sigma_A \;\; i \;\; r}{L} \tag{2.7}$$

where r, the *accuracy* of predicting genetic value, equals the correlation coefficient between predicted and true genetic values of an animal. The *selection intensity* (i) is technically known as the *standardised selection differential.* Selection differential is the difference in measurement between the average of the animals selected for breeding and the average of the population to start with. This measure is in the trait's units; if the trait is litres of milk, the selection differential is in litres. Selection intensity represents the difference between the selected parents ($\bar{x}_{selected}$) and all potential parents ($\bar{x}_{all}$) in phenotype standard deviation units; that is, $i = \frac{\bar{x}_{selected} - \bar{x}_{all}}{\sigma_p}$. The *genetic variation* (σ_A) can be estimated from the between and within family variance components and has an indirect relation with the amount of inbreeding in the population. The *generation interval* (L) is the mean age of parents of all progeny born. With new technologies such as embryo transfer and cloning (Boer 1994), one can decrease the generation interval. Nevertheless, these technologies are new and still expensive. For a bull, the generation interval ranges from 5 to 9 years, whereas for a dam, it ranges from 5 to 6 years. Optimal breeding programs need to balance these components as in Equation 2.7 because they tend to be interdependent. For example, a higher replacement rate decreases generation interval but decreases also selection intensity. Also, a progeny test increases the accuracy (is a gain) but it lengthens the generation interval (is a loss).

Inbreeding

The relationship between animals is measured using the *inbreeding coefficient*, F, which measures the probability that both genes at a locus are identical by descent (Van-Vleck et al. 1987). It represents the probability that two alleles will have arisen from the replication of the same piece of DNA in the common ancestor. These alleles could be at a single locus in one individual (in which case the individuals are said to be inbred) or they may be either one of two alleles present at the same locus in each of two individuals (in which case the individuals are said to be relatives). All those identical by descent alleles are alike in state, that is they occur at the same locus and are of the same type, although the reverse is not true. Therefore, two alleles may be alike in state by chance and not necessarily because they are identical by descent. Therefore, we usually need to define a reference or base population when calculating inbreeding.

If we assume that an animal has an inbreeding coefficient of 50%, this indicates that 50% of all loci in this animal are expected to be identical by descent. Other measures of inbreeding are the coefficient of relationship, f_{xy}, and the coefficient of coancestry, $F_{coancestry}$, or the coefficient of kinship (Falconer 1989). The former measures the likelihood that two individuals carry alleles that are identical by descent. The latter is the probability that the same two individuals will both produce gametes that carry identical by descent alleles. That is, the coefficient of coancestry is half the coefficient of relationship and equals exactly the expected coefficient of inbreeding for the progeny if these two animals were to be mates. Assuming that there is no selection, the inbreeding rate per generation, ΔF, is approximated classically by the following equation (Wright 1931), assuming equal progeny per parent:

$$\Delta F = \frac{1}{8N_m} + \frac{1}{8N_f} \tag{2.8}$$

where N_m and N_f are the number of males and females, respectively, entering the population every year. The average coancestry among a group of offspring can be calculated using the following equation (Wray and Goddard 1994):

$$F_{Coancestory} = X^t A X \tag{2.9}$$

where X is a vector of the proportions of the contributions made by each parent (with male and female part adding to 0.5 each) in the breeding system; that is, the proportion of matings for this

animal, and A is the numerator relationship matrix which indicates the additive genetic relationship among these parents. Henderson (1975b) introduces a recursive function for calculating the matrix A. The algorithm depends on ordering the animals in the pedigree such that parents precede their progeny, then the following rules are applied for animal i where the inbreeding coefficient for animal i is simply; $F_i = a_{ii} - 1$:

- If both parents, s and d, are known, $a_{ji} = a_{ij} = 0.5(a_{js} + a_{jd})$; $j = 1 \ldots (i-1)$ and $a_{ii} = 1 + 0.5a_{sd}$.
- If one parent, s, is known, $a_{ji} = a_{ij} = 0.5a_{js}$; $j = 1 \ldots (i-1)$ and $a_{ii} = 1$.
- If both parents are unknown, $a_{ji} = a_{ij} = 0$; $j = 1 \ldots (i-1)$ and $a_{ii} = 1$.

Mating of close relatives should be avoided in breeding programs since inbreeding increases the fraction of homozygous loci (*ie.* it increases expression of lethal factors). It is further estimated that each percentage of inbreeding leads approximately to a 50 kg weight decrease in milk production (Schmidt and Van-Vleck 1974) and in more general terms, the inbreeding depression on quantitative traits. Mating of unrelated animals always result in non-inbred progeny. If the parents are inbred but are unrelated, then their progeny are not inbred. Different effects of inbreeding are summarised below from (Van-Vleck et al. 1987): -

1. It decreases the frequency of heterozygotes and increases the frequency of each homozygote by half that frequency (*ie.* the population becomes more homogeneous) but it does not change the frequency of alleles. When inbreeding is at its maximum, the population is completely homozygous.
2. It increases the chance of expression of recessive lethal factor, which would allow culling of affected and carrier animals and thereby reduce the frequency of the detrimental genes. However, the cost must be balanced against the potential gain.
3. Line crosses resulting from matings between inbred lines would have mostly heterozygous loci and therefore might be superior to non-inbred animals if there is some form of dominant gene action.
4. It can be used to fix a desirable type (if the reproductive rate is sufficient to allow selection to eliminate the undesirable genes) and to achieve greater uniformity.

5. Inbreeding within a population leads to a loss of genetic variation, and therefore a loss of future reliability to make genetic change.

The expected additive genetic merit, a_i of the progeny i resulting from mating sire s_i and dam d_i can be calculated as (der Werf 1990):

$$a_i = \frac{1}{2}a_{s_i} + \frac{1}{2}a_{d_i} + \phi_i \tag{2.10}$$

$$var(a_i) = \frac{1}{4}var(a_{s_i}) + \frac{1}{4}var(a_{d_i}) + \frac{1}{2}cov(a_{s_i}, a_{d_i}) + var(\phi_i) \tag{2.11}$$

$$var(\phi_i) = \frac{1}{2}[1 - \frac{1}{2}(F_{s_i} + F_{d_i})]\sigma^2_{a_i} \tag{2.12}$$

where ϕ_i is the Mendelian sampling, a_{s_i} and a_{d_i} are the additive genetic values of the sire and the dam respectively, $var(a_s)$ and $var(a_d)$ are the additive genetic variance for both the sire and the dam respectively, $cov(a_s, a_d)$ is the covariance between the additive genetic values of the sire and the dam, $var(\phi)$ is the variance of Mendelian sampling, F_s and F_d are the inbreeding coefficients for the sire and dam respectively, σ^2_a is the additive genetic variance for the population.

2.3 Methods for selection

Dekkers (1998) summarised the current trends in designing breeding programs and suggested that the four main components of a breeding program are the formulation of a breeding goal, methods for evaluation of potential breeding stock, methods for selection, and mating strategies. He states that the crucial criteria for designing breeding programs are the rates of genetic progress and inbreeding, although the overall goal is an economic one. Banks (1988) emphasised two types of decisions: strategic and tactical. Strategic decisions are the choice of a breeding goal, breeds, and selection or crossing system(s). The tactical decisions are the method for selecting animals for mating, and the mating system or the method to allocate animals for mating.

There are a number of methods for selecting animals including: *independent culling levels*, the *classical selection index*- which is also known as *best linear predictor* (BLP), *restricted indices*, *multi-stage index selection*, and the *best linear unbiased predictor* (BLUP). Actually, these methods are used to estimate the genetic merit (breeding values) of animals and then these estimates

are used for the purpose of selection. Before proceeding with a description for each of these methods, some concepts are required.

We must first differentiate between the selection objectives and the selection criteria (Banks et al. 1996; Kinghorn 1995). Sometimes the breeder may wish to optimise a trait that cannot be measured directly, *indirect selection.* In this case, they utilise another trait that is correlated with the one they wish to optimise and can also be measured: for example, using ultrasonic measurement of live animals (selection criterion) to predict carcass quality of slaughtered animals (selection objective).

There are three main types of correlations between traits: genetic, phenotypic, and environmental correlation. Genetic correlation, r_G, is the correlation coefficient between the breeding values of two traits. Phenotypic correlation, r_P, is the correlation coefficient between the observed values of two traits. Finally, the environmental correlation, r_E, is the correlation coefficient between environmental effects on two traits. Let us assume that we have two traits T_1 and T_2, where the first represents the selection objective and the second is the selection criterion. The *correlated response* measures the response's strength on the trait representing the selection objective, when the selection is carried out on the trait representing the selection criteria. The correlated response, $CR_{T_1(T_2)}$, in T_1 from selection on T_2, can be calculated as:

$$CR_{T_1(T_2)} = i_{T_1} \times r_{G(T_2-T_1)} \times \sqrt{h^2 T_1} \times \sqrt{h^2 T_2} \times \sigma_{P,T_1} \tag{2.13}$$

where i_{T_1} is the selection intensity, $r_{G(T_2-T_1)}$ is the genotypic correlation between T_1 and T_2, $h^2 T_1$ and $h^2 T_2$ are the heritability of T_1 and T_2 respectively, and σ_{P,T_1} is the phenotypic standard deviation of T_1.

Independent culling levels

One method of simple selection strategy is by setting a threshold on the trait, and the animal is selected if its value for this trait is higher than the threshold. Another way of applying this strategy is by determining a number of replacements and a certain proportion of animals is chosen on the basis of each trait.

Classical selection index

The classical selection index theory (Hazel 1943) is based on calculating a set of economic weights and then building an index as the sum of the phenotypic values of all traits weighted with the corresponding economic weights. The economic weight is defined as (Banks et al. 1996):

> "the profit margin as a result of a unit increase in the estimated breeding value of a trait while the other traits' genetic merit are held constant".

Given the vector of economic weights, b, the phenotypic variance-covariance matrix of the selection objective's traits, P, the genotypic variance-covariance matrix of the selection criteria's traits, G, and the vector of economic values a, then the selection index I is:

$$I = b^t P \tag{2.14}$$

where the vector of economic weights is calculated as:

$$b = P^{-1} G a \tag{2.15}$$

The genetic gain from using the index can be calculated as

$$Genetic \quad gain = i \times \sigma_I \tag{2.16}$$

where i is the selection intensity and σ_I is the index standard deviation. In this thesis, we are not going to use the classical selection index, and therefore, this index will not be discussed further.

Restricted indices

This is a special case of the selection index where the index is used to maximise a trait while minimising or maintaining the level of another trait (Kempthorne and Nordskog 1959), for example, maximising the milk volume while maintaining the fat percentage. This can be done by simply including the restricted trait, fat percentage, in the objective function and giving it a zero economic value.

Multi-stage index selection

This form of selection takes place in two or more stages. In each stage, the proportion to be selected is set, then a selection index is constructed and the proportion of animals is selected according to their index value.

Best linear unbiased predictor (BLUP)

The selection index theory provides a best linear prediction (Mrode 1996). Generally, BLUP is a selection index (Henderson 1975a), but additionally it corrects for fixed effects (Parnell and Hammond 1985). A multitrait BLUP simply calculates EBVs for each trait. Similar to the classical selection index theory, BLUP ranks the animals according to their EBVs weighted with their relative economic value. BLUP (Mrode 1996) is *best* because it maximises the correlation between the animal's true and predicted breeding value, *linear* since it uses linear models, *unbiased* since the expected EBV which results from BLUP equals the expected true breeding value, and *prediction* since it predicts the true breeding values. BLUP has proven a great success in the dairy industry and other industries such as the pig industry (Gardner 1985).

The yield, y_{ij}, of a cow j in a lactation i can be written as (Jones 1985):

$$y_{ij} = b_i + a_j + p_j + e_{ij} \tag{2.17}$$

where b_i is the fixed effect of the i^{th} herd-year-season, a_j is the additive genetic merit for the j^{th} cow, p_j is the permanent environment effect for the j^{th} cow, and e_{ij} is the error associated with the particular lactation.

In its simple form, a BLUP model for calculating the ABVs for production traits in Australia can be written as (Jones 1985):

$$y = \mathbf{X}b + \mathbf{Z}a + \mathbf{Z}p + e \tag{2.18}$$

where $\mathbf{X}$ and $\mathbf{Z}$ are matrices denoting the herd-year-season and the animal design matrix respectively. The vectors b, a, p, and e represent the herd-year-season fixed effect, the additive genetic merit, the permanent environmental effect, and the estimation error respectively. The solutions

of b, a, and p are given by

$$\mathbf{X}^t\mathbf{X}b + \mathbf{X}^t\mathbf{Z}a + \mathbf{X}^t\mathbf{Z}p = \mathbf{X}^t y \tag{2.19}$$

$$\mathbf{Z}^t\mathbf{X}b + (\mathbf{Z}^t\mathbf{Z} + t\mathbf{A}^{-1})a + \mathbf{Z}^t\mathbf{Z}p = \mathbf{Z}^t y \tag{2.20}$$

$$\mathbf{Z}^t\mathbf{X}b + \mathbf{Z}^t\mathbf{Z}a + (\mathbf{Z}^t\mathbf{Z} + kI)p = \mathbf{Z}^t y \tag{2.21}$$

where $\mathbf{A}$ is the numerator relationship matrix, $t = \frac{(1-r)}{h^2}$, $k = \frac{1-r}{r-h^2}$, r and h^2 are the repeatability (*ie.* the square root of accuracy) and heritability respectively. Quaas (1976) developed a fast algorithm to calculate the numerator relationship matrix inverse. This algorithm was modified by Meuwissen and Luo (1992) whose algorithm was modified again by Quaas (1995). This makes the inverse's calculation for the numerator relationship matrix computationally feasible for very large populations ($>$ 1 million). Additionally, the previous simultaneous equations can be solved by one of the efficient algorithms developed in the literature (Robinson 1981; Schaeffer and Kennedy 1986).

2.4 Selection strategies

There are three decisions to be addressed for cow selection (Schmidt and Van-Vleck 1974):

- Selection for culling.
- Selection for breeding to obtain sons for herd use.
- Selection for breeding to obtain replacement heifer.

The second decision may no longer be important since most farmers depend on artificial insemination instead of his own sires, and not attempt to breed young bulls for AI organisations. If decisions are considered for the short term, selection should be based on the real producing ability. If the program is designed for the long term, selection should be based on genetic values. In practice, a combination of both short and long term objectives is required.

Beard (1987) proposed a linear breeding objective, for the additive genetic merit for lactation yield of the three components of milk (*ie.* fat, protein and carrier), to the Australian industry. The economic weight for a trait is calculated as the difference between the change in returns and change in costs due to a one-unit increase in the trait. With a linear objective function, this

rate of change is valid over the whole domain of each variable. The environmental effects are not considered in the work. In Beard's study, the resultant economic weights for fat, protein and carrier are \$0.8695, \$1.1162 and -\$0.0294 per kg, respectively.

Quinton et al. (1992) present a very useful comparison between different selection methods taking into consideration inbreeding side-effects. They cite that neither Best Linear Unbiased Predictor (BLUP) nor unrestricted selection based on estimated breeding values (which is also based on BLUP) may always be optimal. That is, these selection methods are only suitable for short-term issues.

Meuwissen (1997) introduced a method for maximising the genetic level of selected animals while maintaining an upper bound on the average coancestry to a user-defined value. The index is the breeding values penalised with the coancestry level. The penalty term is represented by the Lagrange multiplier. This index, although it takes the coancestry into account, does not consider the mating pair and consequently it would probably under-estimate short term inbreeding. Such selection methods may therefore lead to more inbreeding. Meuwissen was interested in maximising long term response while maintaining a certain level of new inbreeding each generation. However, as shown in Kinghorn, Shepherd, and Woolliams (1999), even greater responses in mean breeding values can be achieved using both long and short term inbreeding in an MSI in conjunction with the EBV of selected parents. This requires use of mate selection as progeny (short term) inbreeding requires the selection of mating pairs (*ie.* mate selection).

Howarth and Goddard (1998) discuss selection in terms of multiple objectives. They studied two strategies with the farmer optimising two different objectives. In the first strategy (called the specialised strategy), the herd is divided into two sub-herds and each is selected for one of the objectives. In the second strategy, called average, the two objectives average is calculated and the selection is carried out as a single composite objective. The study suggests that the "average" strategy should be used when the objectives are positively correlated and the time horizon to be considered is short-term, or when the herd size limits the specialised strategy usefulness.

Furthermore, specialised strategy generates the greatest response in the short-term, but does this only if the correlations between the objectives are negative (assuming that the economic values of the traits have the same sign). Actually, this result is not new in multi-objective optimisation. The unfavourable correlation merely indicates that there is a conflict between the two objectives. A positive correlation means that there is no conflict between the objectives (*ie.* the maximisation of one objective will maximise the other one). In this case, maximising the average of the two is a reasonable approximation that should result in a non-dominated solution.

Hirooka (1998) illustrates the use of five linear programming based strategies for sire selection. These are *unrestricted* selection, *zero-gain restricted* selection, *non-zero gain restricted* selection, *proportional restricted* selection and desired gain selection. Unrestricted selection is based on the selection index. In the zero and non-zero gain restricted selections, selection is carried out to maximise the selection index and also to maintain the level of a desired trait. For zero-gain, the goal would be to equalise the level of a specific trait within the population. For non-zero gain, the goal would be to maintain a certain level of the difference between the value of sire trait and the mean value for this trait within the set of sires. In proportional restricted selection, the constraint is to maintain the ratio of sires' traits to a certain level. For desired gain selection, selection can be undertaken using zero or non-zero gain restricted selection or proportional selection with the relaxation of the constraint by altering from equality to inequality.

Kinghorn et al. (1999) show that, for certain breeding objectives, optimal selection decisions will depend on how the mates are allocated and the optimal allocation depends on which animals are selected. Consequently, the separation between selection and allocation will result in a suboptimal solution. To summarise, the theory of selection does not consider the interactions among bulls, dams, and the environment, but instead it suggests carrying out the selection on additive genetic values of each animal independently which does not guarantee global optimality.

2.5 Selected recent keywork in mate-selection

A number of algorithms exist for mate-selection (Shepherd and Kinghorn 1999). Generally, there are two steps for implementing the mate-selection problem: developing an objective function,

and developing and implementing a mate-selection algorithm (Kinghorn 1998). In 1985, the first use of optimisation methods in the mate-selection problems appears to have been suggested by Jansen and Wilton (1985) with a conventional linear transportation model for selecting mating pairs. This model easily incorporates different aspects of a real life problem such as inbreeding. However, it does not consider nonlinear genetic objectives.

Kinghorn (1987) compares four mate-selection strategies, three of which are heuristic while the fourth employs linear programming technique. He states that the time for the linear programming calculation increases dramatically with the increase in the population size. The heuristic of sequential allocation of the best pair from the remaining candidates is found to be close to optimal in most cases, although the study is limited to a single generation. However, linear programming computerised solvers have improved dramatically during the last decade. For example, until 1987, Linear programming solvers were using the Simplex method, which is an exponential algorithm (Ami 1993). In 1986, Karmarkar (Hooker 1986) introduced the interior point method which is a polynomial-time algorithm.

Klieve et al. (1994) propose an approximate quadratic programming model for mate-selection using portfolio analysis to construct a quadratic objective for the problem. Additive genetic merit is used as the gain measure (profit) and inbreeding is used as a measure of the risk associated with different levels of merit. Stochastic simulation is used to evaluate different selection strategies with respect to both additive genetic response and inbreeding. The proposed quadratic model results in close to a 50% reduction in inbreeding over the random mating strategy.

In recent work, Kinghorn (1998) proposes clustering to facilitate group mate-selection together with an individual-animal mate selection step for fine-tuning. Cluster analysis is used to form groups of animals within each sex based on nominated factors such as breed, herd, age, and EBV. Mate selection is then performed on groups. The objective is to select 20 sires and 500 dams for breeding, from 816 sires and 1784 dams across 3 breeds. The study reports a considerable reduction in computation time from 394.2 seconds for full mate selection to 0.28 seconds for group mate selection although the cluster analysis took an additional 162 seconds. The maximum number of clusters is chosen arbitrarily as four times the square root of the number of

candidates available. However, the work is certainly important for reducing the search space complexity.

Shepherd and Kinghorn (1994) propose a binary nonlinear programming model for mate-selection over two generations only with cross-breeding. The model accounts for two groups of predicted progeny, those intended for commercial purposes and those for selection and mating. The breeding objective is to maximise the combined return from commercial animals for both one and two generations into the future. The model is limited since it is very difficult to generalise over more than two generations. They also introduced a method to parameterise mate selection.

In summary, the mate-selection problem has not been efficiently solved and a general model to optimise multiple generation seems to be an inevitable requirement within the field.

2.6 Computerised systems for selection in dairy industry

In the literature of animal breeding, decision support systems appear to be mainly management information systems or expert systems and are hardly decision support systems, in the sense used in this dissertation. MacNeil et al. (1998) reviews four decision support systems for the breeding of beef cattle two of which (SIMUMATE and HOTCROSS) are computer programs for prediction and the other two (CROSS-CHOICE and X-BREED) are expert systems. Archer et al. (1998) has suggested the development of a distributed decision support system over the World Wide Web. The proposal discusses the system's functionality but does not show the technical design.

In Canada, interesting research has been undertaken (Lacroix et al. 1997; Wade and Lacroix 1994) which investigated the prediction of milk production for the first lactation of Canadian Holstein dairy cows, using *artificial neural networks* (ANNs). It was found that it is essential to determine which additional inputs add significantly to the prediction process, and which are reasonable in terms of the process's biology. The effect of data pre-processing on the performance of ANNs in predicting milk production is investigated by Lacroix et al. (1997). It is reported that the neural network's ability to predict patterns is highly affected by the class frequencies in

the training set.

The Victorian Department of Agriculture (Bowman et al. 1996) developed a computer program (Selectabull) for selecting the most suitable set of bulls for a farmer's herd and ranking them according to the predictive profitability of each. The profitability is determined according to information submitted by the farmer. Four scenarios are implemented in Selectabull, namely: Manufacturing, Liquid/Quota, Workability, and Altered prices. In each scenario, a selection index is formulated and bulls ranked accordingly. The program also allows for different payment systems. As an example, the breeding objective for Victoria is calculated as $\$ - 0.02 * Milk + \$1.2 * Fat + \$3.9 * Protein + \$4.9 * Survival + \$1.1 * Milkingspeed + \$1.8 * Temperament - \$0.7 * Mature\_body\_weight$. The weights in the objective function are calculated according to the farmer's herd data, milk payment system and the farmers own value judgment if desired.

The difference between Selectabull and the method introduced by Beard (1987) as discussed earlier, is that Beard presented a selection index regardless of the farm information. Selectabull creates a population index to create a team of artificial insemination bulls then it creates a consumer index for each farmer to select from the team. The program achieved its intended goals although it has a number of limitations which motivated this thesis:

- It does not capture important genetic principles such as inbreeding.
- It chooses the bulls for the whole herd without considering the cows' individual characteristics (in short, Selectabull is not designed to solve the mate-selection problem).
- It ranks bulls according to the selected scenario for a breeding objective, without considering the statistical significance of this ranking. It is noted by Bowman et al. (1996) that although the economic weights used for each scenario differed substantially, the correlations between the selection indices are very high.

A system developed by the Machine Learning Research Centre at the Queensland University of Technology called Connectibull (Finn et al. 1996) is designed around a neural network specific for each bull, but has a number of limitations.

- Its employment of a single ANN for each sire does not allow for network generalisation of the effects of sire traits or the general relationship between the progeny and their sires, dams, and the environment.

- It ranks sires for mating with a dam only in terms of predicted production traits of potential daughters (*ie.* similar to Selectabull, it ignores other factors such as inbreeding).

- It is inappropriate for new sires within the artificial insemination program because the number of records available for these sires will be insufficient for training the ANN.

Kinghorn and Shepherd (1999) introduce the *total genetic resource management* (TGRM) approach and propose the *mate-selection index* (MSI) which replaces the classical selection index. MSI is calculated for a mating strategy and not for individual animals. TGRM is a breeding aid program driven by specifying desired outcomes (*eg.* outcomes in genetic gains) (Kinghorn 1999). The user determines the level for each outcome (s)he is satisfied with and the program uses evolutionary algorithms for solving the mate selection problem for one generation while trying to meet the user expectations. Therefore, the program depends somehow on the user to set the goals while these goals may be far from optimal in themselves. This might be a disadvantage but a necessity for the package to optimise the processing time. Also the prediction problem discussed in this thesis is not an issue in TGRM since TGRM does not consider the production values and concentrates instead on the breeding values. TGRM is considered as the state of the art in the field for mate-selection and demonstrates the practical importance of this problem.

2.7 Conclusion

To summarise, the mate-selection problem has not been solved efficiently so far. Current information systems contain the necessary information for the mate-selection problem but none of the existing information systems is qualified to decide on the allocation part except the TGRM system which handle the problem for two generations. This raises two issues: (1) how to design an efficient computer information system for a breeding program, and (2) how to model the multi stage mate-selection problem. The first issue is covered in the next chapter, where it is suggested to integrate knowledge discovery from databases with intelligent decision support systems to solve the problem. The second issue is covered by the remaining chapters where the prediction

problem is investigated and a generic mathematical model for solving the mate-selection problem is proposed and solved.

Part II

Knowledge Discovery in Databases

Chapter 3

KDD-IDSS: A Framework for Integrating KDD with IDSS

The following refereed publication arose out of this chapter:
H.A. Abbass, M. Towsey, G. Finn, and E. Kozan. "A Meta-Representation for integrating OR and AI". International Transactions of Operations Research (ITOR), accepted for a forthcoming issue.

This chapter's main objective is to introduce the proposed information system framework, and to present a new meta-level modular representation for integrating *operations research* (OR) and *artificial intelligence* (AI) models using *constraint logic programming* (CLP). The importance of this language relies on representing a problem generically, and therefore hiding the implementation details from the user.

The chapter begins with a summary of the decision making process (Section 3.1), followed by a literature review of *intelligent decision support systems* (IDSSs) (Section 3.2). In Section 3.3, the process of *knowledge discovery in databases* (KDD) is reviewed and a framework for integrating KDD and IDSS is proposed in Section 3.4. A proposed meta-language for the kernel in the KDD-IDSS is then described in Sections 3.5 and 3.6. Previous work in integrating AI with OR, CLP with OR, and non-symbolic AI with CLP, is presented in Section 3.5 followed by the proposed meta language in Section 3.6. The chapter concludes with an example from the dairy industry (Section 3.7).

3.1 Decision making process

Problems are recognisable through symptoms of abnormal behaviour of system's components. If the symptoms are not recognised early enough, the problem may become a crisis. With an excellent computerised system that has the ability of problem recognition, crises can be evaded. One way to perceive the existence of a problem is suggested by Ata (1988), who defines problem recognition as the process of comparing actual values of some selected variables to their standards. Whenever these standards are violated, the corresponding variable(s) is(are) placed on a list of symptoms. Once symptoms are shown and the problem is identified, one may start by decomposing the problem into sub-problems. By determining the causes and the set of possible actions to solve the sub-problems, the overall problem can be solved. The problem's solution is called the decision.

Problem solving (decision making) is defined when there is a gap between what is desired (the goal state) and what is given (the initial state), and in which the *transitions* that need to be followed to reach this goal are unknown. The process of solving a problem (identifying the transitions) is called *decision making* whereas the process of implementing the solution is *decision taking*. According to the scientific approach in management (Klein 1995), decision making process consists of the following five steps: viz, problem recognition, problem definition, problem formulation, setting goals and designing actions, and evaluation of actions to select the best. The decision maker proposes the selected action to the decision taker who decides whether to take it or not.

As depicted in Figure 3.1 (Trave-Massuyes 1991), there are three types of problems: unstructured, semi-structured, and structured. According to the problem type, the managerial levels are classified into strategic, tactical and operational respectively. From my point of view, resource allocation should not be considered as a managerial level but a common function between the strategic and tactical level. Simon (1960) defines a structured decision as the decision where all the steps required for it can be pre-specified. Simon's definition is influenced by information

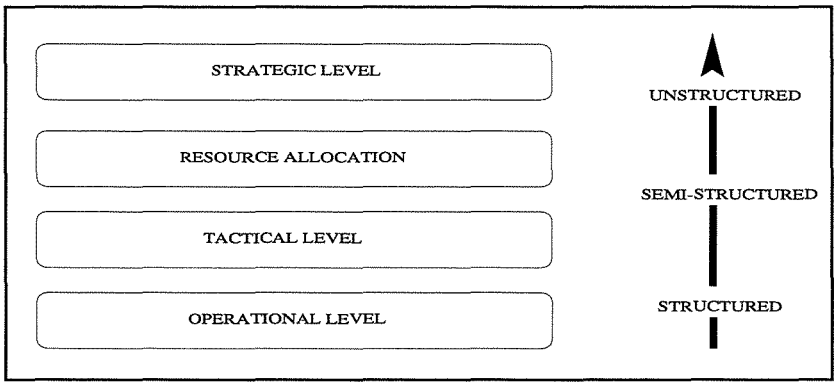

Figure 3.1: The managerial levels

systems whereas most researchers (Fox and Krause 1991; Turban 1990) refer to a problem to be structured if it can be quantified. Tactical problems are semi-structured in that they have both quantitative and qualitative dimensions. DSSs (Turban 1990) provide solutions for the tactical level whereas IDSSs provide solutions for all managerial levels within the system.

3.2 Intelligent decision support system

Decision support systems originated from two research areas during the 1960s. The first is "theoretical studies of human problem solving and decision making" during the 1950s and the 1960s at the Carnegie Institute of Technology. The second is "interactive computer systems" during the 1960s at the Massachusetts Institute of Technology. The two areas became, what was later called in the 1970s, decision support systems. DSS is an integrated information system for decision making.

Despite the emergence of the DSS in the 1970s, presently there is no consensus on the answer to the question: What is a DSS? Some researchers (Sharda et al. 1988) think of a DSS as a collection of theoretical studies driven by a technology push, rather than by a managerial pull. Eierman et al. (1995) propose a theoretical framework for DSS to overcome this claim although the study concentrates on the managerial side without considering the informatics one. To better understand what is a DSS, each of the words Decision, Support, and System is defined.

System A system is mostly defined as a group of components/items that interact together to achieve an overall objective(s) (Gdaellenbach 1995). Each of these components is a system in itself, *ie.* it has sub-components and it has an objective(s). For example, the farm as a system has many sub-components such as the animals, lands, machineries, etc. Each of these sub-components is a system in itself. For example, the animal is a system where its components are organs, genetics, *etc.*

Each component in the system may have local objective(s) which should contribute to the overall system's objective(s). Nevertheless, the component may have an objective that conflicts with the overall system's objective. Unless the component's objective is imposed on the system by a higher power (*ie.* a larger system), it will be rejected. For example, maintaining a certain amount of milk production contradicts the farm objective in maximising the return. Yet the farmer may be obliged to maintain this level of milk production because the Department of Primary Industries assigns to each farmer a milk quota that should not be exceeded. This represents an *external rigid constraint.* If the level of milk production is determined by an internal policy within the farm and it can not be changed, the requirement represents an *internal rigid constraint.* If the internal policy is flexible, (ie. can be changed), the requirement becomes a *soft constraint.* If the policy is to maximise the milk production, without knowing to what extent, it becomes an *objective.* If the milk production level is planned (known), it becomes a *goal.*

Support A computer support system is "a computer system which is placed at the decision maker's disposal who may use data or models to recognise, understand, and formulate a problem, and make use of analytical aids to evaluate alternatives" (Klein 1995). The process of supporting the decision-maker in making a decision, is a continuous process that starts before a decision is made and continues even in the future. Strictly speaking, the system should show some dynamics.

Decision The word decision has been defined and classified in the previous section. Although decision-making and decision-taking may appear to be independent processes, they are not.

Usually in real life applications, some difficulties face the decision-taker when applying the decision. This requires adjusting the decision to cope with the new constraints. The dynamic nature of DSS plays the main role here.

In data mining, DSS has a limited definition where Bigus (1996) defines a DSS as "a query application integrated with a graphical display system". In the literature, the concept of a DSS has evolved. In the early 1970s, Scott-Morton (1971) defined DSS as "decision support systems couple the intellectual resources of individuals with the capabilities of the computer to improve the quality of decisions". As a refinement of Scott-Morton's definition, Little (1970) considers a DSS as "A model-based set of procedures for processing data and judgments to assist a manager in his decision making". In the early 1980s, Bonczek et al. (1980) defined a DSS as: "A computer-based system consisting of three interacting components: 1) A language system - a mechanism to provide communication between the user and other components of the DSS, 2) A knowledge system - the repository of problem domain knowledge embodied in a DSS, either as data or procedures, and 3) A problem processing system- the link between the other two components, containing one or more of the general problem manipulatory capabilities required for decision making".

In the late 1980s, Hicks (1987) defined a DSS as "an integrated set of computer tools that allow a decision maker to interact directly with computers to retrieve information useful in making semi-structured and unstructured decisions". In 1990, Turban (1990) introduced a famous definition of a DSS: "an interactive computer-based information system that utilises decision rules and models coupled with a comprehensive database and the decision maker's own insights, leading to specific, implementable decision in solving problems that would not be amenable to management science optimisation models per se". Lastly, in 1996, Dutta (1996) defined a DSS as "an area concerned with computer based structures and procedures that augment human decision making capabilities". From the previous definitions, the concept of DSS started as a general information system and ended as a structured one in Turban's definition.

To my knowledge, Holsapple is the first to use the term IDSS in his doctoral thesis (Holsapple 1977). The study concentrates mainly on data representation. He suggests having an information base, which is a combination of models and knowledge, where a model, from his point of view,

can be seen as any piece of data. He used network databases which facilitated his concept of a model. The work lacked modularity and interaction and the research in AI at this time was premature.

The term IDSS was not used much since then until 1988. The term *expert decision support systems* was introduced by Sen and Biswas (1985). The term knowledge-based decision support system was suggested by Turban (1990) in 1990. In 1995, Klein (1995) suggested the framework *knowledge-based decision support system* in a work undertaken in France.

IDSS, as used throughout this dissertation, holds a broader scope and deeper dimension. The following definition for IDSS is proposed:

> IDSS is an interactive, structured, and dynamic management information system, that fully or partially automates the decision making process by combining a set of models with a set of symbolic knowledge, while utilising the available databases, in an integrated environment that is capable of reasoning about the decisions it makes.

From the previous definition, 11 keywords are accentuated. **Interactive** reflects the dialogue base component and it places an emphasis on the IDSS's ability to interact with the user and the user role in the system. **Structured** stresses the IDSS modularity. **Dynamical** is achieved in terms of the user feedback and includes the possibility that the system evolves by correcting its mistakes while updating its internal states. **Management information system** highlights the IDSS's original roots and identification as a management information system. **Fully or partially automate** is one of the main features that will be emphasised throughout this work. It represents the IDSS's potential to be an independent environment.

Decision making process places an emphasis on the fact that the purpose of an IDSS is to support or even replace the decision maker although it won't be able to replace the decision taker's perception or job. **Models**, **knowledge**, and **databases** represent the other three components of an IDSS where the first is the dialogue base discussed in the beginning of the definition in terms of the interaction. **Integrated environment** emphasises the fact that the IDSS should not be isolated from, but rather be integrated with, and become a piece of, the surrounded environment. **Environment** represents the information system, the surrounding pieces of softwares, as well

as the decision making environment. Lastly, **reasoning** reflects the system power to rationalise and persuade the decision taker with the decisions it makes.

3.3 Knowledge discovery in databases

Knowledge discovery in databases is simply the task of identifying patterns within a database system. A revised version of the definition in (Frawley et al. 1991) is given by (Fayyad et al. 1996):

> Knowledge discovery in databases is the non-trivial process of identifying valid, novel, potentially useful, and ultimately understandable patterns in data.

Data mining (DM) is a step in the KDD process representing the process of applying the discovery algorithm. There is a common misconception between the use of the term DM and KDD. In academia, DM is a step in KDD (Fayyad et al. 1996) although among the public, DM and KDD seem to be used interchangeably (John 1997). It is becoming apparent that even in modern academia people tend to use the term DM when they mean KDD.

A definition of KDD that suits its intended task within the IDSS paradigm is introduced. KDD is:

> The process of *abstraction* from large databases and the process of searching for patterns and symptoms within the abstracted model.

There are four keywords in the definition: abstraction, search, patterns, and symptoms. The database is a conventional element in KDD.

Abstraction: Abstraction is the process of mapping the system language $\mathcal{L}_1$ to an approximately equivalent language $\mathcal{L}_2$[1]. The mapping is strong when it maps the system while neither losing existing patterns (*completeness*) nor introducing new patterns (*soundness*).

Search: It is more convenient to see the discovery process in terms of search. Therefore, one can measure the complexity, and in turn the feasibility, of the process by studying the search

[1]Formally, Giunchiglia and Walsh (1992) define an abstraction, written $f : \Sigma_1 \Rightarrow \Sigma_2$, as a pair of formal systems (Σ_1, Σ_2) with languages Λ_1 and Λ_2 respectively, and an effective total function $f_\Lambda : \Lambda_1 \rightarrow \Lambda_2$.

space. Most KDD steps can be seen as search-space reduction techniques. For example, the main goal for creating a target data set, data cleaning, and data reduction and projection is reducing the noise in the data and selecting a representative sample which then reduces the search space. The mining algorithm is the search technique used to achieve the overall process objective.

Patterns: A pattern is "an expression, $\mathcal{E}$, in a language, $\mathcal{L}$, describing a subset of facts, $\mathcal{F}_{\mathcal{E}}$, from the total facts, $\mathcal{F}$, which exist in the database" (Fayyad et al. 1996).

Symptoms: Although the symptoms can be seen as patterns, the process of discovering the symptoms has more dimensions than finding simple descriptive patterns. Identification of symptoms is a major task for KDD, if it is the intention to use it for IDSS. The KDD process's role is to clear the noise within the system and discover abnormal signals (symptoms) that may contribute to potential problems.

There are many applications reported in the literature for KDD (Fayyad et al. 1996; Matheus et al. 1996; Smyth et al. 1996; Apte and Hong 1996). Although it seems that there is no general agreement on what the steps for KDD should be, some researchers have tried to structure the KDD process. Fayyad et al. (1996) identify nine steps: application domain understanding, creating a target data set, data cleaning and processing, data reduction and projection, choosing the mining task, choosing the mining algorithm, mining the data, interpreting the mined patterns, and consolidating the discovered knowledge. John (1997) sums up these steps into six, data extraction, data cleaning, data engineering, algorithm engineering, running the mining algorithm, and analysing the results. Regarding the issue of the basis for selecting KDD applications, Fayyad et al. (1996) define four practical criteria and five technical criteria for selecting KDD applications. The former are: the potential for the application's significant impact, no good alternatives exist, organisation support and potential for privacy and legal issues. The latter are, the availability of sufficient data, relevance of attributes, low noise levels in the data, confidence intervals, and prior knowledge.

3.4 A proposed frame for integrating IDSS and KDD

The proposed KDD-IDSS paradigm is shown in Figure 3.2. The conventional IDSS paradigm is extended with a mining base component. This extension influences both the model and knowledge base components. While the set of models and knowledge in the conventional IDSS are static (*ie.* built once and manually updated when necessary), they are dynamic in KDD-IDSS. For example, the mining base continuously builds predictive models and updates the model base with the models it finds. Therefore, if we have a linear regression model in the model base, the parameters in the model are updated every time a change, which may influence this model, occurs in the data. Also the set of rules generated from a mining task may be used to update existing rules in the knowledge base. In short, the system is somehow self-adaptive where the mining base is updating the systems' components based on new changes in the environment. A short description of each component follows.

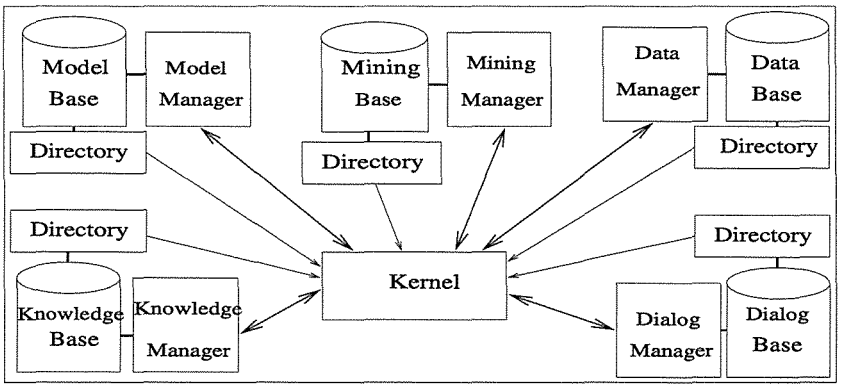

Figure 3.2: The KDD-IDSS paradigm

3.4.1 Database

A set of data that may be directly or indirectly related to the problem. As an example, the ABVs is a datum that is directly related to the problem. The inflation rate, which could be used to predict the prices, is the sort of data which are indirectly related to the problem. A database is usually accompanied by a data manager that organises the way the data is stored, updated, and retrieved. KDD-IDSS interfaces with the database through the data manager and it should not access the data directly for security and efficiency reasons. Also, it can access the data directory

(the logical design and/or meta-data) although it cannot change or add to it.

Rob and Coronel (1997) distinguish between the operational data and DSS data using three criteria: time span, granularity, and dimensionality. DSS data are historical, summarised, and normally multidimensional although operational data are up-to-date, atomic-detailed and one dimension databases. One of the new advances in databases which is motivated by DSS is data warehouses. A data warehouse, introduced by Inman (1994), is defined as: "an integrated, subject-oriented, time variant, non-volatile database that provides support for decision making". Another recent advance in databases is the *on-line analytical processing* introduced by Codd (1993) who defines it as: "on-line analytical processing is the dynamic synthesis, analysis and consolidation of large volumes of multidimensional data". Later, Han (1997) introduced the *on-line analytical mining* which combines on-line analytical processing with data mining techniques.

3.4.2 Model base

A set of models which are required to solve the problem under consideration. Like the database, the set of models in the model base interfaces with the system through a model manager and a description of these models is stored in the model directory.

3.4.3 Knowledge base

A set of facts and symbolic rules about the problem under consideration. The knowledge in an IDSS may be used for the following purposes :-

1. Providing explanation for the system behaviour.

2. Reducing the search space complexity for some models. For example, utilising previous knowledge for decomposing a linear programming problem or eliminating dependent variables and/or constraints from an optimisation model.

3. Generating/expanding the input space for some models. For example, generating or expanding a sample space to be used by neural networks or genetic algorithms.

4. Solving a sub-problem. For example, calculating the inbreeding coefficients.

5. Post-processing of outputs. For example, interpreting the outputs from the linear programming solver.

6. Determining the models' calling sequence. For example, if the decision-maker would like to optimise two years ahead, the calling path may be predictor $\rightarrow$ optimiser $\rightarrow$ predictor $\rightarrow$ optimiser. If the performance in the current year is known, the calling path will be optimiser $\rightarrow$ predictor $\rightarrow$ optimiser.

7. Model selection. For example, according to some criteria either a genetic algorithm module or a conventional optimiser may be called.

8. Helping tool. For example, providing help to the farmer about artificial insemination.

Lastly, rules-weights, probabilities or fuzzy membership functions may be associated with the set of facts and rules in the knowledge base.

As with the previous two KDD-IDSS components, a knowledge base has also a manager which handles the way it is represented and infers new knowledge. Also, items of knowledge are grouped and classified with the description of each group and class stored within the knowledge directory.

3.4.4 Dialog base

The dialog base is the direct outcome of the DSS foundation. Dialog base is based on studies in Human-Computer Interaction. Schneiderman (1987) defines five main styles for human-computer interaction: viz menus, forms, command languages, natural languages, and direct manipulations or graphical interfaces.

1. In menus, the user is restricted with a list of choices and one of them should be selected otherwise the default choice is assumed.

2. In forms, the user is required to fill the parameters within the provided spaces in the form.

3. In command language, the user interacts with the system through a command language in which the language syntax and semantic are predefined.

4. In natural language, the user interacts with the system in a natural language (eg. English) and the system asks the user questions in turn. This type of interface is very complicated to design and/or implement although it is more convenient for novice users.

5. In direct manipulations or graphic based, the user defines the problem in a graphic form (eg. dragging the sign "X" and placing it on a cow shape may be a way of representing a constraint such as the cow is not available for mating).

The actual dialog base may combine some or all of the previous types. The word "dialog base" is used here rather than the conventional word "user interface" to emphasise the idea of interaction in decision support systems. Different studies in human-computer interaction (Molich and Nielsen 1990; Norman 1986; Ravden and Johnson 1989; Scheiderman 1987) concentrates on the user interface as an important part in the program. Norman (1986) associates two properties with an interface language to measure its validity as an interface for a dialog base. The first property is the articularity directness, in which the distance between the physical form, or syntax, of expressions in the interface language and the meaning of the expression is measured. The second property is the semantic directness, in which the distance between the meaning of the input or output expressions in the interface language and the user's intentions or goals, are evaluated.

3.4.5 Mining base

The mining base contains a set of scenarios for the KDD process. These scenarios are a high level description of different pre-designed discovery tasks in the system. The mining base does not store any mining algorithm as these algorithms belong to the model base. Also, database manipulation is no longer the mining base responsibility but rather of the database component. Additionally, data visualisation within the IDSS is the user interface's responsibility and no longer of the mining base concern. In summary, the mining base contains an abstraction of the KDD process for each discovery task. The mining manager organises the storage, retrieval, and updating of different scenarios within the mining base. Furthermore, information about each discovery task is stored within the mining base directory.

3.4.6 Kernel

The kernel is the main interface, sometimes called the operating system, through which all previous IDSS parts interact. This is the most difficult and technical component in the IDSS. To today, there is no generic language for representing the kernel. The contribution of this chapter is to provide such a language for interfacing operations research and artificial intelligence modules within the kernel of KDD-IDSS.

3.5 A meta-language for OR and AI in the KDD-IDSS kernel

The rest of this chapter explores the suitability of CLP as the kernel language for integrating OR and AI. CLP was introduced in 1986 by Jaffar and Lassez (1986), who also developed the first CLP language, CLP(R) (Jaffer et al. 1990). The CLP paradigm overcame the mathematical deficiency in Logic Programming (LP) by introducing new domains (eg. real, rational, boolean, finite trees, etc.) and by defining a suitable set of operands and operations over these domains. The goal of using constraints partially solved the problem of recovery from failure (in conventional logic programming) since constraints can be used in the system as a mechanism to generate a solution space that avoids failure. If the solution space is empty, the system reports failure instead of continuing the search. This reduces the search space as well as providing early detection of failure. CLP continues to be successfully applied to a variety of OR problems such as scheduling (Gosselin 1993), planning (Perrett 1991), quadratic programming (Abbass 1998), multi-criteria decision making (Abbass et al. 1997), and network optimisation (Abbass et al. 1999a; Abbass et al. 1999b). For a typical set of CLP applications, see (Hentenryck 1990). A technical review about the foundations of CLP can be found in (Jaffer and Maher 1994).

In this section, previous attempts to integrate AI with OR, CLP with OR, and non-symbolic AI with CLP, are presented. This section provides the reader with the three dimensions of the integration as a basis for, and to give the motivation for, the meta-language to be illustrated in the following section.

3.5.1 Interfacing AI with OR

Holsapple et.al. (1994) examined this integration and found that both OR and AI involve the use of descriptive knowledge (data and information), embodying measurements, observations, or beliefs about the state of some real or hypothetical world. They conclude that OR focuses on the management of *procedural knowledge*, whereas AI tends to emphasis the management of *reasoning knowledge*. The integration of OR and AI has been discussed in many papers and books such as Barahona and Ribeiro (1990), Donald and Chelsea (1990), Dutta (1996), Holsapple et.al. (1994), Lee (1990), and Moon et.al. (1993). In this chapter, we are taking this research a further step up by formalising the underlying concepts in these works. More specifically, most of these studies were problem specific but a more general frame will be presented here.

Research has been carried out to design frameworks for exchanging data between symbolic AI and quantitative OR techniques. Barahona and Ribeiro (1990) suggest using CLP for integrating expert DSS and OR. This work is not formalised but is illustrated by a conventional example in CLP. Moreover, it considers neither a formal frame for the integration nor the expert DSS components. Turban and Trippi (1990) provide an excellent conceptualisation of the integration between *expert systems* and OR with different concepts for different types of integration although they do not provide an implemental formal frame. Belz and Mertens (1996) combine knowledge base systems with simulation to solve rescheduling problems. They have three main intelligent components: one to initialise the simulation run, the second to supervise it and the third to analyse the simulation output. Their model appears to be well designed for the integration although it was specific to knowledge basis and simulation. A formal generic frame for integrating AI and OR should be developed, on the basis of these studies.

3.5.2 Interfacing CLP with OR

CLP has a pertinent relation to OR as it is centred on constraint solving mechanisms. However, the paradigm is hampered by the conventional limitations of first order predicate logic. CLP implementations can optimise a function with numeric variables but cannot optimise a concept

representation. For illustrative purposes, suppose the concept of customer satisfaction can be represented using the following predicate:-

$$
\begin{aligned}
satisfied(X) :- \\
&customer(X), \\
&budget(X, Y), \\
&like(X, Z), \\
&price(Z, M), \\
&M < Y, \\
&bought(X, Z).
\end{aligned}
$$

This is read as "an object X is satisfied if (X is a customer), (the budget of X is Y), (X likes an object Z), (the price of Z is M), (the price M is within the budget limit of X which is Y) and (X bought the object Z)". Now, suppose that the objective is to maximise $(\forall X, satisfied(X))$, that is to maximise the satisfaction of all customers. The problem can be formulated quantitatively except for the predicate *like* (this problem could possibly be handled by borrowing techniques from decision making, such as utility functions). It is inherent to CLP that it is limited by first order predicate logic (Abbass et al. 1995).

3.5.3 Interfacing CLP with non-symbolic AI

So far, *artificial neural networks* (ANNs) have not been sufficiently considered in a CLP environment. Montesi (1996) proposes a model for representing ANNs within CLP in which current CLP semantics for equations are used to represent the network as a system of equations. The network is trained outside the CLP paradigm and then embedded within CLP. This would have been more efficient if CLP were capable of training the network so that retraining would not require updating the CLP program.

To my knowledge, the use of a *genetic algorithm* (GA) solver in CLP has not been considered. We consider that it has potential to enrich the power of CLP paradigms by making all successful applications of GA available to CLP as well.

3.6 The proposed meta language

This section essentially describes the details of the proposed language used for the integration. First, the concept of decision making is structured using CLP-like syntax, allowing the decision to be decomposed by CLP into a set of component predicates. Each component predicate can be an optimisation, a neural network, natural language, or knowledge based system. The component predicates are then constructed as a set of predicates in CLP-like language. In this way, all component predicates are abstracted and, consequently, the meta-language is independent of any specific implementation. Therefore, the intelligent problem solving process can be illustrated using a three layered system.

- The first layer is the meta-language, used to abstract a particular problem.
- The second layer is a classifier system, where a decision tree is employed to identify the type of models required to solve the problem. For example, if the user requires the optimisation of a problem, the classifier system will analyse the objectives and constraints to determine the more appropriate optimisation model.
- The third layer is the detailed implementation level where the actual coding for each algorithm is implemented.

This chapter is concerned only with the first layer. The second layer is assumed to be a single path decision in this thesis, whereas the third layer is the subject of the remaining chapters.

3.6.1 Formalising the concept of a decision in KDD-IDSS

From the previous section, we have seen that the KDD-IDSS is very flexible since it isolates the mechanism for solving a problem from the problem formulation stage. Therefore, if the problem complexity increases and the KDD-IDSS requires more sophisticated techniques to handle the new version of the problem, all it requires to do is to call a different appropriate solver. For example, calling a Simplex solver for a medium size linear programming and calling an interior-point solver for a large size linear programming.

Given a set of decision variables *Variables*, a set of constraints *Constraints*, and a set of criteria *Objectives*, a decision requires the values of *Variables* to meet the set *Constraints* and optimise the set *Objectives*. Formally speaking, the decision can be defined as a function $D = select(Variables, Solution, Objectives)$ where $Solution = solve(Variables, Constraints)$, that is the predicate *solve* returns a set of solutions where the predicate *select* evaluates them and selects the optimal. This definition illustrates two important stages in problem solving. The first stage is the process of finding a set of feasible solutions (ie. alternatives) represented, using the predicate *solve*/2 (*name*/n means that the predicate *name* has n arguments). This is equivalent to the feasibility stage in OR. The second stage is equivalent to the optimality stage in OR where the elements in the set resulting from the feasibility stage are evaluated, and the one which best satisfies the criteria is selected using the predicate *select*/3.

We then have to define the criteria's nature. For global optimality, one can implement the predicate *select*/3 either by using exhaustive search or formulating the problem as an optimisation model. Both ways are computationally expensive but optimisation is much less though, since it does not exhaust the search space but instead searches a sub-space in a systematic way until the optimal solution is reached.

The second type of criteria that can be used is the concept of satisfaction (introduced by Simon (Simon 1960) and also called the Simonian philosophy), which attempts to satisfy a set of goals rather than to optimise a set of objectives. The goal is always partially satisfied to some aspiration level (possibly 0%) so that one or more solutions always exist. If the constraint system is not satisfied, the solution space will be empty. Bearing this difference between a constraint and a goal in mind, a satisfaction problem can be handled using an updated version of the techniques used for solving a normal optimisation problem by adding a free variable to each goal equation. Then, for any set of decision variables' values, a goal equation is satisfiable for some values of its free variable. The free variables can be minimised later subject to a set of user preferences (eg. goal programming). Therefore, we may have a multi-dimensional objective, as well as goals that may be prioritised - see (Abbass 1994) for an update to the CLP language, SICStus, to handle goal programming problems. Next, we can rewrite the literal *Solution* as follows: $Solution = solve\_new(Variables, Constraints\_rigid \cap Constraints\_soft)$. Therefore, in

recasting the optimisation model as a satisfaction model *Constraints* became *Constraints_rigid* and *Objectives* became *Constraints_soft*. Further, *solve*/2 for optimisation is a special case of a new predicate *solve_new*/2 for satisfaction, where

$solve(Variables, Constraints) = solve\_new(Variables, Constraints\_rigid \cup \phi), Constraints = Constraints\_rigid.$

where Φ is the empty set. Accordingly, for the satisfaction models the decision can be redefined as:

$D = select(Variables, Solution, Objectives)$, where
$Solution = solve\_new(Variables, Constraints\_rigid \cup Constraints\_soft)$.

We consider all possible cases.

$D = select(Variables, \phi, Objectives) = \phi \rightarrow$ No Solution
$D = select(Variables, Solution, \phi) = Solution \rightarrow$ Satisfaction problem
$D = select(Variables, Solution, Objectives) = X, Solution \neq \phi$ and $X \neq \phi$.

If the cardinality of X is 1, we have a unique solution; otherwise, we have multiple solutions. However, the set D is not necessarily finite - it may indeed be uncountable infinite, in which case we may represent D by a set of constraints called the "most general form".

The set of constraints over D can be further classified as predicates and functions. Predicates are functions that take the values 0 or 1 (ie. true or false) and are used extensively to represent symbolic knowledge. Unfortunately, propositional logic is insufficient to represent some important relations. For example, in order to generalise the concept of grand-fatherhood we need to enumerate propositions for this relationship in the world. In first-order predicate logic, grand-fatherhood can be expressed more naturally in terms of the concept of fatherhood: $grandfather(X, Y) : -father(X, Z), father(Z, Y)$. This means that if X is the father of Z and Z is the father of Y, then X is the grandfather of Y where there is an implicit use of universal quantification. For all people X, Y, and Z require only that the concept father is defined in

context. We can still represent the relation grandfather using an integer model. For illustration purpose, let $grandfather(X,Y)$, $father(X,Z)$, and $father(Z,Y)$ be denoted as $C1, C2$, and $C3$ respectively. Now, the predicate can be represented as $C1 = \frac{1}{2}(C2 + C3)$, where $C1, C2$, and $C3$ are binary variables. Yet we are unable to represent here the universal quantifier, although the binary variables can be related to domains where the universal quantification is applied on the domain. Finally, we can rewrite our definition for a decision in the following way:

$D = select(Variables, Solution, Pred\_Objectives \cup Func\_Objectives)$ where
$Solution = solve\_new(Variables, Pred \cup Constraints\_rigid \cup Constraints\_soft)$.

This definition represents an abstract problem representation. The *Pred_Objectives* component, representing the qualitative objectives, can be handled by the knowledge base, whereas the *Func_Objectives* component, representing the quantitative objectives, can be handled by the optimisation module.

3.6.2 The relationship between the proposed concept of a decision and previous ones

The goal of using the Prolog environment as a kernel for DSS is not new. Fox (1991), presents a DSS based on first order predicate logic (FOPL) in medicine. He does not employ optimisation techniques to build the DSS. Lee et.al. (1996) propose the following representation for *quantitative/qualitative constraint satisfaction* (QQCSP) problem, $W = [E, R\_E, F\_E] \cup [N, R\_N, F\_N] \cup [E \cup N, R\_EN, F\_EN]$; where E is a set of symbolic objects, R_E and F_E are sets of relations and numeric functions on the set E respectively, N is a set of symbolic objects, R_N and F_N are sets of relations and numeric functions on the set N respectively, and R_EN and F_EN are sets of relations and functions on both E and N. They also compare the use of mixed integer programming and constraint logic programming and conclude that models are easy to represent and modify and the solution could be partial if we used CLP instead of mixed integer programming. Actually, their representation of QQCSP is not sufficient to handle our definition of a decision since we need to incorporate the evaluation criteria (the objective function). Therefore, we have updated Lee at.al. representation to

$D = select([E \cup N], Solution, Pred\_Objectives \cup Func\_Objectives)$

where

$Solution = [E, R\_E, F\_E] \cup [N, R\_N, F\_N] \cup [E \cup N, R\_EN, F\_EN]$.

This illustrates the need for a method of evaluating the alternatives for solving the QQCSP. This can be handled quantitatively, provided there are no symbolic objectives; that is, the term $Pred\_Objectives$.

In the rest of the chapter, the (-) sign denotes that the variable is not instantiated and is used as a predicate output. The (+) sign denotes that the variable should be instantiated before it is used as an input to the predicate.

3.6.3 Using CLP to integrate AI and OR

The purpose of this section is to abstract different functionalities in AI and OR systems using CLP. Thus, each component predicate hides the implementation details for some complicated functionalities. A problem is then defined by a synthesis of these predicates in a CLP-like program.

Optimisation

Optimisation models can be considered as a predicate $optimise(-Variables, +Objectives, +Constrc$ that takes as its inputs the set of uninstantiated variables $-Variables$, constraints $+Constraints$, and objective $+Objective$ and $-Variables$ will be instantiated with a solution if exists. In the optimisation model, the input space is known and the solution algorithm uses the projective transformation to generate the null space. This can be written in CLP-like syntax as: -

$$optimise(-Variables, +Objectives, +Constraints) : -$$
$$solve(-Variables, +Constraints, -Solution\_space),$$
$$select(-Variables, +Objectives, +Solution\_space),$$
$$bind\_multioptimals(-Variables).$$

Predicate *optimise* fails if the predicate *solve* fails and succeeds otherwise. Elements in the list $-Variables$ will be instantiated if the *select* predicate returns a single solution, otherwise it is a representation of the objective function's projection on the null space. In any case, the predicate *bind_multioptimals* binds the values in $-Variables$ to a single value (using a pre-specified heuristic) and with backtracking, more optimal solutions can be generated.

Neural networks

In *multi-layer feed-forward artificial neural networks* - also known as *multi-layer perceptron* (MLPs) - we sample both the input and output spaces and seek a representation of the mapping function from the input space to the output space. MLPs can be represented as $MLP(+Inp\_samp, +Out\_samp, +Architecture, -Function)$ where an input space's sample $+Inp\_samp$ and the corresponding output space $+Out\_samp$ is input to the network, as well as the the network topology represented by $+Architecture$. The predicate MLP returns the set of parameters for the function $-Function$. The optimisation module can be used for optimising the weights during the network training. MLPs can be represented as :-

$$MLP(+Inp\_samp, +Out\_samp, +Architecture, -Function) : -$$
$$generate\_parameters(+Architecture, -Parameters),$$
$$train(+Inp\_samp, +Out\_samp, +Architecture, -Parameters),$$
$$construct\_function(+Architecture, +Parameters, -Function).$$

The predicate *generate_parameters* generates the set of parameters (weights and biases) $-Parameters$ associated with a pre-defined architecture $+Architecture$. The predicate *train* undertakes the training process of the MLP then passes the set of instantiated parameters to the predicate *construct_function* which synthesises the function and returns it as a mathematical representation of the neural network.

Expert systems

A *production system* is a concept inspired by human psychology where human cognition is viewed as a set of condition-action pairs called *productions*, and the programs that control human behaviour are organised as production systems. A production system consists of a production memory, a working memory, and a control strategy. Pairs of condition-action rules are stored in the production memory. In the working memory, the world's current state is matched against the rules. The control strategy is the mechanism of firing (activating/executing) a rule. Production systems are general, simple, and flexible frameworks for search with the advantage that knowledge is separated from control. This framework is language independent and the explanation can be carried out very easily. Knowledge based systems can be represented as $expert\_system(+Initial\_state,\ +Kb,\ +Goal\_state,\ -Path)$.

The inputs are a set of rules $+Kb$, the initial state $+Initial\_state$ and a goal state $+Goal\_state$. The function returns the reasoning or the path of rules, $-Path$, taken to reach the goal state from the initial state. Expert systems can be represented using the following predicate :-

$$
\begin{aligned}
&expert\_system(+Initial\_state, +Kb, -Goal\_state, -Path) :- \\
&\quad expert\_system\_con(+[Initial\_state|Kb], +Initial\_state, -Goal\_state, [], -Path).
\end{aligned}
$$

$$
\begin{aligned}
&expert\_system\_con(+Kb, +Goal\_state, +Goal\_state, +Path, -Path). \\
&expert\_system\_con(+Kb, \_, -Goal\_state, +Path\_in, -Path\_out) :- \\
&\quad select\_a\_rule\_to\_fire(+Kb, -Fired\_rule), \\
&\quad fire\_rule(+Fired\_rule, -New\_state), \\
&\quad remove\_rule\_from\_kb(+kb, +Fired\_rule, -New\_kb), \\
&\quad expert\_system\_con(+[New\_state|New\_Kb], +New\_state, +Goal\_state, \\
&\qquad +[Fired\_rule|Path\_in], -Path\_out).
\end{aligned}
$$

The predicate *expert_system_con* expands the predicate *expert_system* for programming reasons. The predicate *select_a_rule_to_fire* selects a rule from the knowledge base according to the conflict strategy. The predicate *fire_rule* fires the selected rule which is also added to the reasoning path. Note that the predicate *expert_system* can be implemented in various ways; this is an example for illustration. The predicate *optimise* can be called from within two predicates,

select_a_rule_to_fire and *fire_rule* predicate. Sometimes, the rules in the knowledge base are weighted, with the weights possibly derived from an optimisation problem, and influence which rule should be fired. Firing a rule may also cause the optimisation module to be called.

Natural language processing

There are eight different types of linguistic analyses used in natural language processing: prosody, phonology, morphology, lexis, syntax, semantics, pragmatics, and world knowledge. Prosody deals with rhythm and intonation; phonology with sound patterns; morphology with the smallest grammatical units in the language (morphemes) contributing to the formation of words (un-, anti, etc.). Lexis is the set of tokens that constructs the language and constitutes the dictionary. Syntax deals with the structure of words and the rules of grammar. Semantics is concerned with the sentences' and lexis' interpretation. Pragmatics is the discipline that discusses contextual aspects of the sentences or the lexis such as speech roles. World knowledge consists of cultural aspects which are conducive to understanding the language.

In its simple form, natural language processing can be viewed in terms of a function $f(sentence, rules, dictionary)$ that takes as its inputs the sentence to be analysed, the set of rules and the dictionary and outputs a suitable analysis for the sentence. The output may be "valid" or "invalid" if this sentence is valid/invalid in the language. If valid, further output of the sentence's "grammatical structure", a sentence's "semantic representation", and a "reply" might be generated. Each of these outputs requires a corresponding suitable analysis. For example, the second output will need lexical and syntax analysis whereas the fourth output will need in addition semantics and pragmatics. Problems, up to the stage of pragmatic analysis, can be written as: -

$$
\begin{aligned}
&nlp(+Sentence\_in, -Sentence\_out) :- \\
&\quad parse(+Sentence\_in, -Sentence\_structure\_in), \\
&\quad semantic(+Sentence\_structure\_in, -Semantic\_representation\_in), \\
&\quad pragmatic(+Semantic\_representation\_in, -Semantic\_representation\_out), \\
&\quad semantic(-Sentence\_structure\_out, +Semantic\_representation\_out), \\
&\quad parse(-Sentence\_out, +Sentence\_structure\_out).
\end{aligned}
$$

The predicate *parse* either takes a sentence and returns its structure or vice-versa. The predicate *nlp* always succeeds as long as *parse* succeeds and fails only when *parse* fails. At this stage, we assume that it is the predicate *parse* responsibility to determine not only the sentence structure but also whether or not the sentence is defined as a valid sentence within the semantic structure. The predicate *semantic* either takes a sentence structure and returns its semantic structure or vice-versa, while the predicate *pragmatic* takes a semantic representation and returns an equivalent semantic representation, sometimes in a different representational language. Notice that we may have all or part of the process (ie. predicate *nlp*). Additionally, we can embed within the natural language process an optimisation problem, by adding to the *semantic* predicate the capability to extract the correct inputs for the predicate *optimise*, where the semantic representation here is the mathematical model. Furthermore, the predicate *optimise*'s output can be passed back to the user as a reply. In this case, the *nlp* predicate is used as a front-end to the optimisation problem. To demonstrate how to implement a "what-if" analysis scenario using optimisation techniques (sensitivity analysis) in our proposed framework, we employ:

$$
\begin{aligned}
&what\_if(+Sentence, -Output) :- \\
&\quad parse(+Sentence, -S_1), \\
&\quad semantic(+S_1, -[Variables, Objectives, Constraints]), \\
&\quad optimise(-Variables, +Objectives, +Constraints), \\
&\quad semantic(-S_2, +[Variables, Objectives, Constraints]), \\
&\quad parse(S_2, -Output).
\end{aligned}
$$

Additionally, the optimisation predicate can use the expert system predicate to select from a multi-optimal set, or to prioritise goals in goal programming, etc. Furthermore, when solving a decomposed problem, neural networks can be used to relate the outputs of various sub-problems to predict the master problem's objective value. However, it is difficult to envision a role for natural language processing within the optimisation problem. The previous definitions of subsystems components in terms of CLP predicates, set a structure for calling any component from the others. CLP is the centre around which these predicates are built.

3.7 An example of the language

In mate-selection, the farmer collects all possible data about the herd, and the system is required to construct a mating plan which optimises a set of genetic and economic objectives. The database contains data about the farm and any other related data. The model base contains solvers for the optimisation models, and prediction's models. The knowledge base has production rules, which are generated from the mining base. The mining base contains a scenario for mining the database to find out why a specific mating should take place. The kernel contains the meta-language for controlling the overall process. A scenario for this work will now be presented as an example.

Assume that the farmer would like to optimise the mating-plan for a single year. The system will first submit a query for solving the problem as follows:

$?mating\_plan(+My\_farm, -Plan).$

where the system is asking for a mating plan for the database called My_farm. The $mating\_plan/2$ predicate is expanded into its components.

$$
\begin{aligned}
&mating\_plan(+Farm, -Plan) :- \\
&\quad get\_mating\_objective(-Current\_objective), \\
&\quad get\_farm\_cows(+Farm, -Cows), \\
&\quad get\_farm\_bulls(+Farm, -Bulls), \\
&\quad generate\_MLP\_data(+Cows, +Bulls, -Inp\_samp, -Out\_samp, -Architecture), \\
&\quad MLP(+Inp\_samp, +Out\_samp, +Architecture, -Function), \\
&\quad predict\_all\_combinations(+Cows, +Bulls, +Function, -Progeny), \\
&\quad generate\_mating\_constraint\_system(+Cows, +Bulls, +Progeny, \\
&\qquad +Current\_objective, -Objectives, -Constraints), \\
&\quad optimise(-Variables, +Objectives, +Constraints), \\
&\quad semantic(-S, +[Variables, Objectives, Constraints]), \\
&\quad parse(+S, -Plan).
\end{aligned}
$$

that is, $get\_mating\_objective/1$ retrieves the objective, which the farmer wishes to optimise, from

the database. Then, *get_farm_cows*/2 and *get_farm_bulls*/2 retrieve the cows' and the bulls' data from the farm database. After that, *generate_MLP_data*/5 retrieves from the database a pre-defined architecture and a data set required to construct a regression model, which will be constructed by the neural network predicate $MLP/4$. Once the regression model is constructed, *predict_all_combinations*/4 enumerates all possible mating pairs and uses the regression model to predict the progeny's outcome. We may not need to predict all possible combination of matings because it is an expensive task; therefore, we just predict a combination when it is required. The predicate *generate_mating_constraint_system*/6 generates the mathematical model using the set of *cows*, *bulls*, and *progeny*, in addition to the farmer objective. The model is solved using *optimise*/3, an English-like sentence's structure is constructed using *semantic*/2, and *parse*/2 puts the sentence together to construct the mating plan.

This scenario illustrates one of the practical applications of the meta-language defined in the previous section. It shows the power of using such language in problem solving since the problem is described in a natural and abstract way, leaving out the details to the system. The system analysts need not worry about which model is solving the mathematical model or which learning algorithm is used to train the neural network. Instead their only concern would be to worry about the problem's logical description.

3.8 Conclusion

In this chapter, a generic information system framework for integrating IDSS and KDD is proposed to automate the breeding program's design process. The kernel of the proposed framework requires a generic meta-language for problem representation. Therefore, a meta-level modular language is presented using constraint logic programming as a framework for integrating operations research and artificial intelligence modules. The language provides a high-level abstract description of the steps needed to solve problems that require operations research and artificial intelligence modules. The proposed language extends previous attempts in the literature with a general problem independent syntax. The potential usefulness of this language is demonstrated using an example from the dairy industry. In this example, it is shown that the language is

generic and isolates the user from the implementation's details.

This chapter emphasises the first thesis sub-objective; designing a generic kernel for the KDD-IDSS. The rest of the thesis will discuss the second and third thesis sub-objectives; that is, discovering patterns in the dairy database using KDD, and formulating and solving the mate-selection problem.

Chapter 4

Mining the Dairy Database

The following refereed publications arose out of this chapter and the contributions of the other authors are excluded except where it is mentioned otherwise

**) P.E. Macrossan, H.A. Abbass, K. Mengersen, M. Towsey, and G.D. Finn. "Bayesian neural network learning for prediction in the Australian dairy industry", Lecture Notes in Computer Science LNCS1642, Intelligent Data Analysis, pages 395-406, 1999.*

**) H.A. Abbass, W. Bligh, M. Towsey, M. Tierney, and G.D. Finn. "Knowledge discovery in a dairy cattle database: (Automated knowledge acquisition)", Proceedings of the Fifth International Conference of The International Society for Decision Support Systems (ISDSS'99), Melbourne, Australia, July, 1999.*

In the design of KDD-IDSS, a distinction must be made between the single-value of a prediction technique and the reasoning surrounding the prediction. Point-estimation methods are commonly used to construct a single-value prediction model, whereas interval estimation methods are useful to generate the reasoning behind the prediction. The problem under scrutiny is the prediction of a progeny's productivity given information about its sire, dam, and environment. This chapter investigates the suitable technique(s) for point and interval estimation for this problem. Multiple linear regression is compared against artificial neural networks, for point-estimation. For interval estimation, RULEX and C5 are compared. The Bayesian unsupervised learner Autoclass is used to cluster the continuous variables as a pre-processing step for interval estimation. The relative success of each method in satisfying the objectives of a breeding program is presented.

This chapter is structured as follows: The function estimation problem in KDD-IDSS is presented in Section 4.1 followed by *multi-layer feed-forward artificial neural networks* (MLPs) in Section 4.2, *Autoclass* as a Bayesian classifier in Section 4.3, and *decision trees* (DTs) in Section 4.4. Although ANNs are biologically motivated, this thesis will emphasise their application as non-parametric statistical methods, rather than their biological foundation. The dairy database is then presented in Section 4.5, and the point-estimation experiment in Section 4.6, followed by the interval-estimation experiment in Section 4.7. Conclusions are drawn in Section 4.8.

4.1 The function estimation problem in KDD-IDSS

In practice, two types of estimation methods are used during building real-life KDD-IDSSs: point and interval function estimation. The former, normally known as prediction, maps an input vector to a single point in the output space. The latter, usually referred to as classification, maps a vector of intervals in the input space to an interval in the output space. Both methods have advantages and disadvantages within an KDD-IDSS.

Point function estimation methods are normally useful in an application where a single predicted value is required, usually for subsequent inclusion in some numerical function. Examples may include using the predicted value as a coefficient in the objective function of a linear programming model, or in the domain of animal breeding, using the predicted value in the calculation of a selection index. The main disadvantage of point estimation methods is their inadequacy for use in reasoning through the application of IF-THEN rules. IF-THEN rules need intervals in both the rule's body and head. Without intervals, the number of rules would be unwieldy, due to the necessity of attaching some meaning to each point in the problem space.

Interval function estimation methods, overcome this disadvantage of point estimation methods by dividing the continuous input and output spaces into intervals that can then be related to meaningful symbolic descriptions, such as "low" and "high". Such descriptions facilitate the reasoning associated with a particular result. Using the dairy industry domain for example, a predictive IF-THEN rule might be "if the dam production figure is low then the daughter production figure

is low". The word "low" here may have different meanings or bindings for each attribute about which we are reasoning, such as milk volume. Nevertheless, it is necessary to hide the bindings from the user to overcome the problems associated with the interpretation of rigid boundaries. For example, the interval for "low" production might be determined by an expert opinion to range from zero to 5000 litres of milk. If the boundaries were visible to the user, he or she may ask what difference there exists between a dam that produces 5000 litres to one that produces 5001 litres? Is one litre of milk production sufficient to consider the dam producing 5001 litres as no longer a "low" producer? These types of questions can be avoided by assigning labels to intervals.

Although in practice the questions are avoided, in reality the problem of arbitrary interval ranges and class boundaries remains, and a number of potential problems exist with the interval approach. First, if the predictor and response variables are continuous, a break-point or boundary must be imposed between intervals to implement the IF-THEN criterion. This break-point might be subjective - perhaps based on prior or expert opinion - or objective, based on some statistical or information theory methods. However, experts potentially suffer from criticisms of bias, while objective methods may be influenced by a high correlation with other predictor variables. In either case, the correlation between two variables may be reduced to a weak or non-existent one, for example, with a change in the break-point. The second disadvantage is that the information lost in the collapse of a continuous variable through a binary split, may be greater than the benefit gained from the resultant inference.

This chapter aims to compare two methods that predict progeny performance. Specifically, the contribution of MLPs and DTs in solving the estimation problem in general is investigated. The output of the adopted point estimation model may be used as input to the optimisation model in KDD-IDSS. The output of the adopted interval estimation model may be used to generate the knowledge base in a KDD-IDSS.

4.2 Artificial neural networks

The human brain has been a mystery that motivated the research into biologically plausible models for modeling the brain functionalities. The biological models are called neural networks and their counterparts in computer science are called *artificial neural networks* (ANNs). The fundamental nature of either artificial or biological, neural network's concept is a large number of neurons can display an emergent intelligence based on the approach in which the neurons are interconnected (Towsey 1998). The fundamental cognitive activity of a neural network is pattern recognition and completion (Bechtel and Abrahamsen 1991). The cognitive model of neural network is also known as *connectionism* and from the computer science perspective as *parallel distributed processing.* The difference of ANNs from other computational systems is that their data structure mimics some known features of the human brain anatomy and physiology. Nevertheless, ANNs, although they are inspired by biological neural networks, do depart from them for practical reasons.

The first idea for computational or neural modeling originated with the work of McCulloch and Pitts (1943). They introduced the concept of a simple type of *linear learning machines*, the *perceptron*, which is a simple thresholding element with some inputs, each of which is either 0 or 1. Each input is modified by a multiplicative weight and the output of the perceptron is 1 if the weighted sum of its inputs exceeds a certain threshold; otherwise 0. By relaxing the constraint that each input is binary, the perceptron is in essence a linear function capable of discriminating linearly separable objects in R^n. Each input vector is called an *instance*, or *input pattern*, and the output is called an *output pattern.* The input-space is usually referred to as the *feature space* and the output-space as the *hypothesis space.* The process of updating the weights until the network correctly maps the inputs to the outputs is called *learning.* The data are usually partitioned into three sets, a set for learning the function called the *training set*, a set for validating the model called the *validation set*, and a set for testing the generalisation of the model called the *test set.* By *generalisation* we mean the ability of the *learning machine* (*ie.* the learning algorithm) to give the correct output on unseen data (data which are not included in the training or validation sets). The learning machine is said to *over-fit* if it is biased towards the training set instead of learning the underlying function; that is, it memorises the training set and does not generalise over the feature space.

There are two categories of learning algorithms: *supervised* and *unsupervised* (Hertz et al. 1991). In supervised learning, the output is used as a teacher which guides the network while it is updating its weights, by comparing the network output against the original output. In unsupervised learning, the output is not available and the network is required to generate such an output. For example, if we would like to group (*cluster*) cows together but we do not know on what basis we should discriminate between cows, the task is an unsupervised learning one. However, if we choose to discriminate between cows based on their level of milk production, and we wish to identify from a set of features the causes that a cow is a low milk producer, then the task is a supervised learning task. The process of assigning a cow to a class is called *classification* or *interval estimation* while the process of determining the expected milk of the cow is called *prediction* or *point estimation*. An ANN which contains a number of intermediate layers (maybe 1) of perceptrons is called *multi-layer perceptron* (MLP).

Fifteen years following the discovery of the perceptron, a substantial number of studies has been undertaken. Some noteworthy works are listed below:

- Von Neumann (1956) introduced the idea of redundancy to remove (prune) unreliable parts of the network,
- Rosenblatt (1962) proved the convergence of a learning algorithm for an ANN without intermediate layers, and
- Minsky (1967) showed that ANNs are capable of universal computations,
- The abundonment of the computer science community to the field of ANNs for almost 20 years following the book *Perceptrons*, by Minsky and Papert in 1969, that showed the perceptron is incapable of learning some types of functions such as XOR.

Research in ANNs flourished again with the introduction of Back-propagation (BP), a learning algorithm for adjusting the weights of an MLP until the network approximates the underlying function, by Rumelhart et al. (1986). Essentially, BP was developed by Werbos (1974) and then developed independently by Rumelhart group. This algorithm will be explained in more detail later in the section.

For the sake of brevity, the limitations of ANN technology are explained. The obvious criticism for non-symbolic techniques, including ANNs, is that the technique is a black box; that is, the knowledge incorporated into the model (network) and the reasoning underlying the technique's behaviour are opaque to the user. In some domains, this is a severe disadvantage since the decision cannot be explained in a rational way to the decision taker. The attempts to overcome this limitation culminated in several techniques for rule extraction from ANNs (see (Andrews et al. 1995)).

4.2.1 The structure and training of MLPs

We may define an ANN by a graph: $G(N, A, \psi)$, where N is a set of neurons (also called nodes), A denotes the connections (also called arcs or synapses) between the neurons, and ψ represents the learning rules whereby neurons are able to adjust the strengths of their interconnections. The neuron receives its inputs (also called activation) from an external source or from other neurons in the network. It then undertakes some processing on this input and sends the result as an output. The underlying function of a neuron is called the activation function. When the inputs to the neuron are the outputs of other neurons, the activation, a, is calculated as a weighted sum of these outputs in addition to a constant value called the bias. From herein, the following notations will be used for a single hidden layer MLP:

- I, J, and K are the number of input, hidden, and output units respectively.
- $\mathbf{X}^p \in \mathbf{X} = (x_1^p, x_2^p, \ldots, x_I^p), p = 1, \ldots P$, is the pth pattern in the input feature space $\mathbf{X}$ of dimension I, and P is the total number of patterns.
- $\mathbf{Y}^p \in \mathbf{Y}$ is the corresponding class of pattern $\mathbf{X}^p$ in the hypothesis space $\mathbf{Y}$.
- w_{ij} is the weight connecting input unit i, $i = 1 \ldots I$, to hidden unit j, $j = 1 \ldots J$.
- w_{jk} is the weight connecting hidden unit j to output unit k, $k = 1 \ldots K$.
- $H_j(\mathbf{X}^p) = \sigma(a_j)$; $a_j = \sum_{i=0}^{I} w_{ij} x_i^p$, $j = 1 \ldots J$, is the hidden unit's output j corresponding to the input pattern $\mathbf{X}^p$, where a_j is the input to hidden unit j, and $\sigma(.)$ is the activation function that is taken in this thesis to be the logistic function where $\sigma(z) = \frac{1}{1+e^{-Dz}}$, with D the function's sharpness or steepness and is taken to be 1 unless it is mentioned otherwise.

- $\hat{Y}_k^p = \sigma(a_k)$; $a_k = \sum_{j=0}^{J} w_{jk} H_j(\mathbf{X}^p)$ is the output of unit k in the output layer, $k = 1 \ldots K$, for the input pattern $\mathbf{X}^p$.

The network topology may vary considerably from an application domain to another (since the topology defines the underlying function the network tries to approximate). Typical ANNs architectures are shown in Figure 4.1.

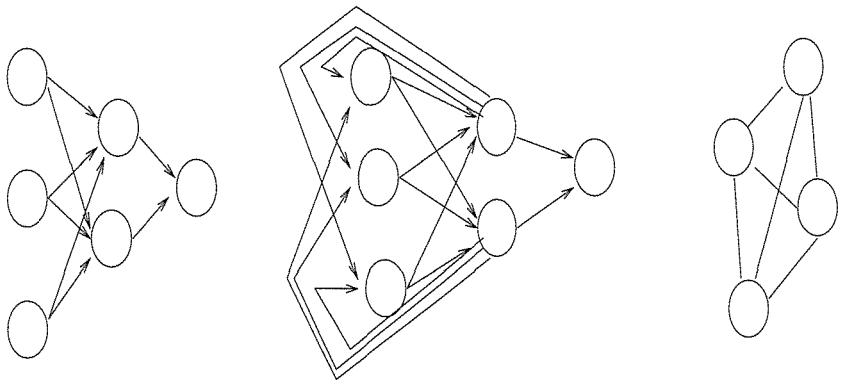

Figure 4.1: Three different ANN's architectures.

left, a three-layer feedforward neural network; *centre*, a recurrent neural network with a feedback from the hidden units to the inputs; and *right*, a fully connected Hopfield neural network.

MLPs from statistical perspective

MLPs are in essence non-parametric regression methods which approximate underlying functionality in data by minimising a loss function. This task can be defined formally as follows:

Given a set of input-output ordered pairs, $< \mathbf{X}^p, Y^p >$, the task of an MLP is to find a set of parameters, α (*ie.* weights and biases), which approximates the underlying data distribution. The network task is achieved by the minimisation of a risk function (Vapnik 1995) of the form,

$$R(\alpha) = \int L(\mathbf{Y}, f(\mathbf{X}, \alpha)) dF(\mathbf{X}, \mathbf{Y}) \tag{4.1}$$

where $L(.,.)$ is a loss function, $F(.,.)$ is a joint probability distribution function of occurrence of observation instances, and $f(., \alpha)$ is the mapping function of the MLP for parameter set α. The data are presented to the network and the risk function is approximated empirically by summing over all data instances. The common loss functions used for training an MLP are the *quadratic*

error function and the *entropy*. The *back-propagation* (BP) algorithm (Rumelhart et al. 1986) is commonly used for training the network.

Back-propagation

The risk function is approximated by summing over all input patterns. Therefore,

$$R(\alpha) = \sum_{p=1}^{P} \sum_{k=1}^{K} (Y_k^p - \hat{Y}_k^p)^2 \tag{4.2}$$

The BP algorithm uses the gradient of the risk function to change the parameter set α until the risk is minimum. The algorithm is given in Figure 4.2. For a complete description for the derivations of this algorithm, see (Haykin 1999).

---

until *termination condition is satisfied*
  foreach $(\mathbf{X}^p, Y^p)$ *in the training set*
    inject the input pattern $\mathbf{X}^p$ *into the network*
    calculate the network output values for hidden units, $H_j(\mathbf{X}^p)$*, and output units* $\hat{Y}^p$
    foreach *output unit* k, $r_k = \hat{Y}_k^p(1 - \hat{Y}_k^p)(Y_k^p - \hat{Y}_k^p)$ *where* r_k *is the rate of change in the error of unit* k.
    foreach *hidden unit* j, $r_j = H_j^p(1 - H_j^p)\sum_{k=1}^{K} w_{jk} r_k$ *update each weight in the network*
      $w_{ij} \leftarrow w_{ij} + \Delta w_{ij}$
      $w_{jk} \leftarrow w_{jk} + \Delta w_{jk}$
        where
          $\Delta w_{ij} = \eta r_j a_{ij}$
          $\Delta w_{jk} = \eta r_k a_{jk}$
          η *is the learning rate; the length of the step to be made in the search space*

Figure 4.2: The Back-propagation algorithm.

4.2.2 Rule extraction from artificial neural networks: RULEX

Rule extraction from neural networks helps provide explanations for the behaviour of neural networks. The advantages of rule extraction include (Andrews and Diederich 1996):

- it helps to integrate connectionist systems with symbolic ones,
- it is a powerful tool for automated knowledge acquisition,

- the rules sometimes generalise better than the networks from which they are extracted, and
- the rules may expose previously un-recognised dependencies.

There are many techniques for rule extraction; in this thesis only one technique is described, RULEX, which is used during the experiment. For a set of techniques, the reader may use Andrews and Diederich (1996) as a guide. RULEX (Andrews et al. 1995) is a technique developed at QUT's Machine Learning Research Centre, for extracting rules from neural networks that have been trained by the "rapid-backprop" algorithm. Each node in the network is a local response unit (LRU). The network is trained by adjusting the centres, widths and steepness of the bumps (*ie.* intersections of sigmoid functions in n dimension) to minimise the output error. When training is complete, rules are extracted by a direct encoding of the response field of each hidden unit.

There is an additional rule-refinement phase which reduces and simplifies the rules to increase comprehensibility. The three refinement operations are negation, elimination, and absorption. If all possible values of an attribute but one occur within a rule, negation of the absent value is used instead. If all possible values of an attribute make the corresponding ridge active, that attribute is eliminated because it does not contribute to discrimination. Absorption refers to the elimination of an attribute's negation when it is redundant.

In general, RULEX depends on the LRUs' configuration. This has the disadvantage of rules being local by definition and global structure may be undetectable. Nevertheless, these techniques are easy and fast to train and the resulting refined rule set can be accurate and concise. Andrews et al. (1995) compared a number of rule extraction techniques and found that RULEX alone did not need parameter initialisation.

4.3 Bayesian clustering

Bayesian clustering is based on Bayes rules in statistics. Bayes theorem provides a unique approach to assign a degree of plausibility to any proposition, hypothesis, or model. Note that

the Bayesian approach is not directly concerned with model creation, but with assessing a model with respect to the available data and knowledge. Surprisingly, it can be proved, in a strict mathematical sense using Cox-Jaynes axioms, that Bayesian inference is the only consistent way of reasoning in the presence of uncertainty (Baldi and Brunak 1999). To describe the Bayesian inference, let us assume a set of data D, and a model $M = M(w)$ parameterised over the set of parameters W. The Bayesian theorem states that

$$P(M|D) = \frac{P(D|M)P(M)}{P(D)} \tag{4.3}$$

where, $P(M)$ is called the prior probability and represents our belief or knowledge about the model, $P(D|M)$ is called the likelihood and represents the probability that this data set is driven from the model, M, $P(D)$ represents the probability of the data, and finally $P(M|D)$ represents the posterior probability or our updated belief in the model. It is usually difficult to calculate $P(D)$ and since it is independent of any model, M, we can rewrite Bayesian theorem as

$$P(M|D)\alpha P(D|M)P(M) \tag{4.4}$$

Now, let us assume two models that we would like to compare, M_1 and M_2, and that we lack any prior knowledge about the problem; therefore it is reasonable to assume each is equally likely, giving $P(M_1) = P(M_2) = 0.5$. In this case, maximising our posterior probability $P(M|D)$ will be equivalent to maximising the likelihood $P(D|M)$. This approach is called *maximum likelihood* approach. It is worth mentioning that if the error in the data follows a standard normal distribution, a neural network with quadratic error function is equivalent to the maximum likelihood approach (Mitchell 1997).

Autoclass

Autoclass (Cheeseman and Stutz 1996) is an unsupervised clustering algorithm based on Bayes theorem. In unsupervised learning, the task is to discover clusters or classes in the data rather than generate class descriptions from labeled examples as in supervised learning. Autoclass is based on the classical finite mixture distribution, which is a two-part model. In the first part, given a data set and a probability density function, one seeks the posterior parameter values that give the maximum interclass mixture probability that an instance belongs to the class. Instead of

doing this, Autoclass seeks the full posterior probability distribution of these parameters. Thus, if we denote the set of classes by C, and the parameters of the class distribution by θ, and the class probabilities by π, the objective is then to find the posterior probability distribution by maximising the following likelihood

$$p(x|C) = \iint p(\theta, \pi|C)p(x|\theta, \pi, C)d\theta d\pi \tag{4.5}$$

In the second part, one seeks the appropriate number of classes, or equivalently the posterior distribution of the number of classes C:

$$p(C|x) = \frac{p(C)p(x|C)}{p(x)} \tag{4.6}$$

The remaining question to be answered is: what is the most appropriate probability density function that represents a class. Autoclass assumes a Gaussian distribution in the case of continuous attributes and Binomial for discrete attributes. The user sets a maximum number of classes which is used as an upper bound by Autoclass. The prior distribution of the classes is derived from the data itself. After the clustering is complete, a hierarchical model is derived by finding the dependencies among the parameters.

4.4 Classification decision trees

DTs are either univariate or multivariate. *Univariate decision trees* (UDTs) approximate the underlying distribution by partitioning the feature space recursively with axis-parallel hyperplanes. The underlying function, or relationship between $\mathbf{X}$ and $\mathbf{Y}$, is approximated by a synthesis of the hyper-rectangles generated from the partitions. *Multivariate decision trees* (MDTs) have more complicated partitioning methodologies and are more computationally expensive than UDTs. The split at a node in an MDT depends on finding a combination of attributes that optimally (or satisfactorily) partitions the input space. This is a very expensive process, since finding a single linear hyperplane which optimally splits the data at a node is an NP-hard problem (Hoeffgen et al. 1995). Nevertheless, an extensive literature for MDTs (see (Sreerama 1997) for a review) exists documenting attempts to find better ways to combine attributes for splitting, to

prune resultant trees, to deal with missing values, and to handle noisy inputs.

Optimisation and statistical methods play a significant role in the determination of MDTs. Breiman et al. (1984) was one of the first to develop methods for generating MDTs by introducing *Classification and Regression Trees.* Brown and Pittard (1993) use a linear programming formulation for each class at each node to determine the variable mix required to optimally split the data. However, this is computationally very expensive. Another attempt was made to formulate MDTs as an optimisation model, by Bennett (1994), which has the advantage of determining all splits simultaneously but with the disadvantage of a resultant non-linear optimisation model. The model solutions in cases of high dimensionality are very difficult and time consuming especially since the objective function is usually non-differentiable. In an attempt to overcome this drawback, a Tabu-based algorithm was suggested by Bennett and Blue (1997) in which a re-formulation of the optimisation model is employed to optimise an existing decision tree rather than generating the tree from scratch. Although the model results in a tree with higher accuracy, it does not guarantee a globally optimal tree structure.

C5

C5 (Quinlan 1997), is a supervised-learning decision tree classifier and an enhancement of the earlier version C4.5 (Quinlan 1993). C5 maximises information gain by branching on that attribute which minimises an entropy function. Most importantly, the default parameter settings for C5 are extremely robust in that, they yield good results for a wide range of problem domains and data sets. Having constructed a complete decision tree, C5 proceeds to extract rules. It suffers the disadvantage that if the data is separable by a function such as $x < y$ for two attributes x and y, 100% accuracy is achievable only with a tree of infinite size because C5 synthesis the decision boundary with hyper-rectangles. Furthermore, redundancies in the training set can cause difficulties for C5.

4.5 The dairy database

The objective of the experiments to be presented is to predict the expected progeny milk production from any given mating. The original data set is obtained from the *Australian Dairy Herd Improvement Scheme.* The data set consists of 48 text files containing both raw and summary data of milk production in dairy herds around Australia. The subset of data used in this thesis applies to Holstein dairy cattle from the State of Victoria. Records are filtered to remove those containing incomplete milk volume, fat and protein data, those records that lacked sire and dam information, and also to include only those records where the number of test days per lactation is greater than seven (a reliability measure). An exploratory data technique, principal component analysis [1], is carried out on the resultant data set to determine which variables are to be included in the final feature set. This analysis indicated that some of the variations in the predictor can be explained by the dam season of calving. As a result, the final feature set includes *dam second lactation milk volume* SLMV, sire ABV for milk, dam herd mean milk yield excluding first lactation and dam season of calving (autumn, summer, winter, spring).

Data pre-processing

It is common practice in the dairy industry to correct milk production values for age (Schmidt and Van-Vleck 1974), since mean production yields vary with age at lactation. The production traits are corrected for the effect of age and the season of calving is included as an input since it was difficult to identify its trend from the available data. Consequently, the features dam SLMV and the daughter *first lactation milk volume* (FLMV) required to be corrected for age. The correction factor, CF, is calculated as

$$CF = \frac{MV(mature)}{MV(group)} \tag{4.7}$$

where $MV(mature)$ is the average milk volume (MV) of all mature cows aged 5 to 7 years (when production is at a peak) and $MV(group)$ is the average MV of all cows in the age group being corrected. Cows are grouped by age where each age group is of one year length. In Figure 4.3, the average dam *lactation milk volume* (LMV) as a function of age (in months) before

[1] The principal component analysis was done by Paula Macrossan (2000).

and after age correction is shown. As seen by comparing Figures 4.3a and 4.3b the correction removes a small nonlinear trend thereby representing the effect of cow age on its milk production.

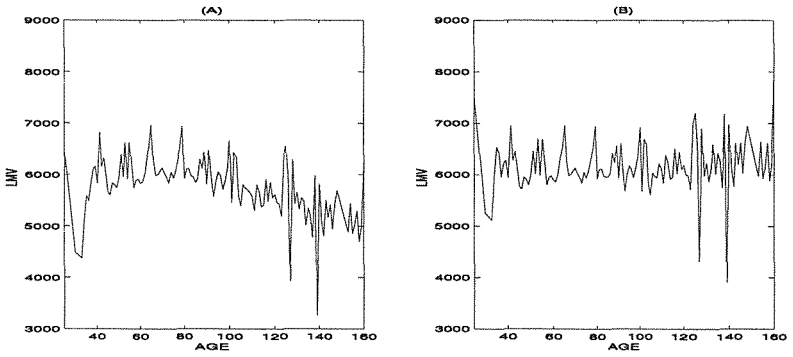

Figure 4.3: The impact of age (in months) correction on dam LMV.

At left (A) Dam LMV before age corrections as a function of age in months. At right (B) Dam LMV after age corrections as a function of age in months.

In the final data set, dam season of calving is represented as a sparse-coded variable. The continuously-valued variables (representing dam, sire and herd information) are linearly transformed to values between zero and one.

The final data set contained 20682 data records in the training set, and a further 5204 records in the test set. These two sets were obtained by random sampling from the database. A validation set as well as cross-validation are not required here since the amount of data is large compared to the number of hidden units tested. As mentioned in (Berthold and Hand 1999), over-fitting is not an issue in these circumstances. There are seven input variables, representing the following variables:

1. Dam herd mean milk yield excluding first lactation
2. Dam SLMV
3. Sire ABV for milk yield

4-7.Dam season of calving (autumn, summer, winter, and spring).

Each record also contains the daughter FLMV, the variable for prediction.

4.6 Experiment (1): Mining for predictive models

Mining for predictive models is not an easy task for two reasons. (1) There is no general algorithm that can ascertain in advance whether linear model is more suitable than a nonlinear one for the data. (2) Even if the data fits a nonlinear model better than a linear one, "what is the best nonlinear model that should be used to fit the date" is still a hard question. Consequently, experimenting with techniques such as neural networks appears to be a logical solution even though they are computationally expensive.

The problem of predicting the daughter milk production from sire and dam production records appears to have many characteristics which might make an ANN solution more attractive than that obtained using other machine learning paradigms. ANNs have a tolerance to both noise and ambiguity in data (Widrow et al. 1994). The dairy data, like other agricultural data, is noisy due to many random and unpredictable effects. The database contains indicators representing genetic and environmental influences (Finn et al. 1996). ANNs are able to approximate non-linear relationships between sets of inputs and their corresponding sets of outputs (Lacroix et al. 1994). The dairy data could be expected to better fit a non-linear model. The ability of ANNs to generalise well (Rumelhart et al. 1994) and to learn concepts involving real-valued features (Dietterich 1990) are potential advantages with this exercise, since the predicted daughter responses are continuous variables.

4.6.1 Methods

Two approaches are compared here: MLPs and multiple linear regression (MLR) (Abbass et al. 1999). There are many statistical techniques more sophisticated than MLR such as generalised linear models (Berthold and Hand 1999). However, MLR was used as a simple benchmark technique. The full training set of 20682 records is used for model's construction in both approaches, with the full test set of 5204 records used to verify the predictions obtained.

The data are modeled using an MLP with seven input units, one for each data input, one hidden layer of $1, 2, 3$, or 4 logistic units, and a single output unit representing daughter first milk

yield. The four MLPs' architectures with a single hidden layer of $1, 2, 3$ or 4 units, with logistic activation functions are trained ten times with different weight initialisations for 20,000 epochs and tested on the test set every 50 epochs using a learning rate of 0.03 and zero momentum[2]. The average of the ten weight initialisations is reported for each network. The software employed for MLP is *Tlearn* (MIT 1997) in batch mode. The predictions of the different methods on test data are compared using the correlation between the network actual output and the target output, mean error, *root mean square error* (RMSE), and absolute error; where the error is the difference between the network actual output and the target output.

4.6.2 Results

Artificial Neural Networks

The correlations between the target value of daughter first milk yield and the value predicted by the MLP for network architectures of one, two, three, and four hidden units, and also the error components for the predictions, were all the same (see Table 4.1).

Table 4.1: Performance of MLP for different number of hidden units on the dairy database.

Number of Hidden Units	1	2	3	4
Correlation	0.76	0.76	0.76	0.76
Mean Error	0.01	0.01	0.01	0.01
RMSE	0.06	0.06	0.06	0.06
Mean Abs Error	0.05	0.05	0.05	0.05

Correlations between the target values of daughter first milk yield and the predicted values, the mean of the error, RMSE, the mean absolute error for MLP. The standard deviations are excluded since they are approximately 0 for all experiments. The differences are found to be insignificant between the different performances.

Linear Regression

All seven covariates of interest were employed for MLR[3]. However, dam season of calving (spring) was eliminated due to the dependency generated in the data from the binary encoding of the

[2]A momentum is sometimes used to accelerate the convergence of BP (Haykin 1999).

[3]The MLR experiment was undertaken initially by myself and repeated independently by Paula Macrossan (2000).

seasonal effects.

MLR gave similar results as MLP. The correlation coefficient between the target values of daughter first milk yield and the predicted values was 0.76, the error mean was almost 0, the RMSE 0.06, and the mean absolute error 0.05.

4.6.3 Discussion

Two main conclusions arise from the studies carried out in this experiment. First, the data fits a linear model (MLR) as accurate as a nonlinear model (MLP), which did not improve the predictive accuracy of the model. Therefore, both approaches (MLP and MLR) are equivalent in terms of their predictive accuracy on the dairy data, as indicated by a test of correlation coefficients between target and predicted value of daughter first milk yield.

Second, it is apparent from this study that each different method has its own distinctive advantages. On the one hand, linear regression provides straightforward descriptions of the relationship being portrayed, and some quantification of the importance of each input attribute, by way of the coefficients in the linear equation. On the other hand, the MLP approach supported our belief that the data fits a linear model as good as a nonlinear one.
Experimenting with neural networks is a very costly task in terms of both time and computational complexity. Usually, people see this as a disadvantage of neural network although (Elder and Pregibon 1996) shows that this is an advantage. In their comments about neural networks Elder and Pregibon wrote,

> "... they appear so over-parameterised, and the weight adjustment procedure is a local gradient method, sequential, and interminable (leading to a crude type of regularisation wherein moderating the runtime becomes the principle way to avoid overfit). However, these weaknesses cancel somewhat, as the slow, local search does not allow the excess of parameters to be overfit easily. ... The danger of overfit can depend on the training duration, since many random node weights lead to essentially linear functions (nodes operating in either the middle or an extreme of the sigmoid) and such linear functions are absorbed by subsequent layers. Only as nodes get pushed into the curved part of the sigmoids during training do many parameters

become active. (This may explain the common observation that the performance of an MLP on a problem is often surprisingly robust with respect to changes in its network structure)."

4.7 Experiment (2): Automated knowledge acquisition

In KDD-IDSS, the system requires continuous source of knowledge to update the knowledge base. The expert is a subjective and expensive source of knowledge. This experiment's objective is to use machine learning tools to automate the knowledge acquisition process. The experiments are carried out in two stages. In the first stage, the attributes are discretised using Autoclass (presented in Section 4.3). In the second stage, a comparison between RULEX (presented in Section 4.2.2) and C5 (presented in Section 4.4) is carried out to select the suitable technique.

4.7.1 Methods

In this experiment, the four attributes used in the previous experiment, herd not FLMV (*ie.* all lactations excluding the first), sire ABV milk, dam SLMV, and the season of calving, are preserved here. Autoclass is used to categorise daughter FLMV. However, Autoclass defines its clusters using the mean and standard deviation of a Gaussian distribution. In order to obtain the boundary, b, between any two classes having means μ_1 and μ_2 ($\mu_2 > \mu_1$) and standard deviations σ_1 and σ_2 respectively, the following formula was used (Abbass et al. 1999):

$$b = \mu_1 + \sigma_1 \times \frac{(\mu_2 - \mu_1)}{(\sigma_1 + \sigma_2)} \tag{4.8}$$

Then, the sets of rules obtained are compared using two types of inputs representation, continuous and discrete, using Autoclass and two types of rule induction algorithm, RULEX and C5. Comparisons are based on three criteria: the rule set accuracy, the number of rules and the average number of antecedents per rule. Rule set accuracy is determined by calculating the average of precision and recall for each output class. Precision is defined as the percent of positive cases correctly classified in the class to the total number of cases classified as positive. Recall is the percentage of positive cases correctly classified in the class to the total number of positive cases originally belonging to this class (Witten and Frank 2000).

The number of rules and average number of antecedents per rule affords an objective measure of rule set comprehensibility. Comparisons between C5 and RULEX are difficult in this regard because, unlike C5, RULEX combines rules using disjunctions and negations. To make comparisons more fair, the rule refinement step of RULEX is reversed by decomposing disjunctive rules into simpler elemental rules.

For example, a rule of the form "if (V or W) and (X or Y) then Z" consists of four elemental rules after Boolean operator distribution. A trade-off between the three criteria reflects generalisation. For example, in the average class for the discrete case in Table 4.4, the accuracy of RULEX at 48% is 12% more than C5 but at the cost of having additional 121 rules (134 versus 13). In knowledge basis, it is important to balance between the accuracy of prediction and comprehensibility or the number of rules used for prediction. Accordingly, we claim that C5 is better in this case than RULEX even though it has slightly lower accuracy.

4.7.2 Results

Table 4.2 presents a summary description of the categorisation of continuous variables resulting from Autoclass. The attributes average herd MV, dam SLMV, sire ABV and daughter FLMV are divided into 6, 5, 7, and 3 categories respectively. Accuracy and comprehensibility results for the rule sets extracted by C5 and RULEX are shown in Tables 4.3 and 4.4 for continuous and discrete inputs respectively.

In most cases, the accuracy of the rule sets produced with continuous and discrete inputs are similar. Only in one discrete case is there a major difference (the "average" class in Table 4.4). There are however, quite distinct differences in the numbers of rules. RULEX produces more rules when the inputs are discrete (Column 4 in Table 4.4) and C5 produces more rules when the inputs are continuous (Column 4 in Table 4.3). Accordingly, in terms of comprehensibility, RULEX has the advantage with continuous data, whereas C5 holds advantage with discrete data.

Table 4.2: Summary of data categorisation using Autoclass.

Class	Upper bound	Frequencies (%)
Herd milk Average Volume		
Low	4794	24
Below Average	5306	20
Average	5613	12
Above Average	5986	14
High	6300	10
Very High	N/A	20
Dam SLMV		
Low	4346	13
Below Average	5039	14
Average	5830	20
Above Average	6350	13
High	N/A	40
Sire ABV Milk		
Very Low	278	02
Low	623	12
Below Average	735	11
Average	842	12
Above Average	1108	24
High	1475	26
Very High	N/A	13
Daughter FLMV		
Low	4632	44
Average	5624	30
High	N/A	26

Table 4.3: Results of classification with continuous inputs.

Output Class	Classifier	accuracy	number of rules	average number of antecedents per rule
Low (44%)	RULEX	75	2	3
	C5	75	28	4
Average (30%)	RULEX	39	4	3
	C5	41	43	5
High (26%)	RULEX	53	3	3
	C5	65	21	3

Table 4.4: Results of classification with discrete inputs.

Output Class	Classifier	accuracy	number of rules	average number of antecedents per rule
Low (44%)	RULEX	76	36	3
	C5	76	12	2
Average (30%)	RULEX	48	134	4
	C5	36	13	3
High (26%)	RULEX	66	30	3
	C5	65	6	2

4.7.3 Discussion

The human domain expert preferred the rule sets derived from discrete variables even in cases where there are more rules for discrete. The domain expert's opinion is that, where rules are to be used to support a decision, it is semantically easier to employ category labels rather than numeric intervals. For example, a rule such as "if the herd milk average is low then the daughter milk production is low" is easier for the user to appreciate than "if the herd milk average $<$ 4794 then the daughter milk production $<$ 4632". Additionally, the expert noted that rules with discretised variables remain valid even if improvements in breeding and management practices increase absolute animal yields and therefore change the boundaries determining the categories. Consequently, we judge that discrete inputs are more convenient in our case.

As noted above, C5 performs better than RULEX on the discretised data, the preferred method of data representation by the domain expert. This leads to selection of C5 as the classifier for the knowledge base in the KDD-IDSS. RULEX has the disadvantage that it is restricted to learning two class problems. For problems with more than two classes as in this case, a separate neural network must be trained for each class, adding considerably to the computation effort, therefore each record is classified a number of times. Where contradictions exist among a record's intermediate classification, some sort of conflict resolution is required. C5 by contrast can handle classification problems involving large numbers of classes. The data discretisation did not vary the prediction accuracy much. Therefore, the results are insensitive to discretisation.

To summarise, C5 appears to be more suitable than RULEX for this application, because it

produces smaller and more comprehensible rules sets and performs well with a default set of parameters, therefore obviating the need for user interaction. The set of rules generated by C5 are included in Appendix A. We may notice that the order of rules is important in C5.

4.8 Conclusion

In this chapter, two experiments are carried out to estimate the expected daughter's milk volume giving information about the dam, sire, and environment. The estimation problem scrutinised in the two experiments is investigated as both a point and an interval estimation problem.

This chapter emphasises the second thesis sub-objective; discovering patterns in the dairy database using KDD. The experiments presented in this chapter inspire a new method for generating multivariate decision trees. This new method is the context of the next chapter. The rest of the thesis will then discuss the third thesis sub-objectives; that is, formulating and solving the mate-selection problem.

Chapter 5

C-Net: A new Method for Generating Non-deterministic and Dynamic Multi-variate Decision Trees

The following refereed publication arose out of this chapter and the contribution of the other authors are mentioned in the relevant places

H.A. Abbass, M. Towsey, and G. Finn. "C-Net: A Method for Generating Non-deterministic and Dynamic Multi-variate Decision Trees". Knowledge and Information Systems (KAIS), Springer-Verlag, accepted for a forthcoming issue.

Although ANNs are universal function approximators, their "black box nature" (that is, their lack of direct interpretability or expressive power) limits their utility. In contrast, UDTs have expressive power, although usually they are not as accurate as ANNs. An improvement, C-Net, is proposed for both the expressiveness of ANNs and the accuracy of UDTs by consolidating both technologies for generating MDTs. Additionally, a new concept, recurrent decision trees, is introduced, where C-Net uses recurrent neural networks to generate an MDT with a recurrent feature. That is, a memory is associated with each node in the tree with a recursive condition which replaces the conventional linear one.

Furthermore, it will be shown empirically that, in test cases, the proposed method achieves a balance of comprehensibility and accuracy intermediate between ANNs and UDTs. MDTs are

found to be intermediate since they are more expressive than ANNs and, more accurate than UDTs. Furthermore, in all cases MDTs are more compact (*ie.* smaller tree size) than UDTs.

The importance and motivation of this algorithm are introduced in Section 5.1 followed by previous work in combining ANNs and DTs in Section 5.2 and the C-Net algorithm in Section 5.3. In Section 5.4, experimental results and comparisons are presented and the recurrent version of C-Net is then scrutinised in Section 5.5. Conclusions are drawn in Section 5.6.

5.1 Motivation and importance of C-Net

Since the introduction of *constraint logic programming* in 1986 (Jaffer and Lassez 1986), constraints have become an acceptable form for both knowledge representation and reasoning. In some domains, the representation of attributes in symbolic format is neither efficient nor natural. For example, in the galaxy classification problem of Sreerama (1997) it is more natural to relate coordinates of the image with a mathematical relation. Additionally, one can sometimes interpret the constraints as logical formulae when the variables are binary. For example, if X_1 and X_2 are two binary variables, $X_1 + X_2 \geq 1$ is equivalent to the logic function *OR*. This motivates the research into multivariate classification trees where a condition on a node is represented by a linear combination of some, or all of the attributes.

In this chapter, a simple novel algorithm, C-Net, is proposed for generating MDTs from ANNs. In the implementation, Quinlan's C5 (an enhancement of his earlier C4.5 (Quinlan 1993)) is employed for constructing UDTs. The algorithm employs the gain ratio calculated by C5 to compute a composite variable, to engineer a decision split at a node. The algorithm has three stages. Firstly, a single hidden layered ANN is trained on a suitable training set until performance is deemed to be satisfactory. Secondly, the training set is presented once more to the now-trained ANN but the outputs of the hidden units become the input feature vector to C5, with the target output still playing its usual role in defining the hypothesis space. Thirdly, the UDT in the new feature space of hidden unit outputs is readily converted to an MDT in the original feature space X.

In Figure 5.1, we show the ANN and C-Net for a hypothetical problem. The purpose of this figure is to illustrate how the back-projection is calculated. Also, it shows that C-Net offers a simple graphical representation of the ANN. The MDT is effectively a transformation applied to the non-separable function generated by the ANN to approximate it with piecewise linear functions. The resultant MDT is easier to interpret than the corresponding ANN.

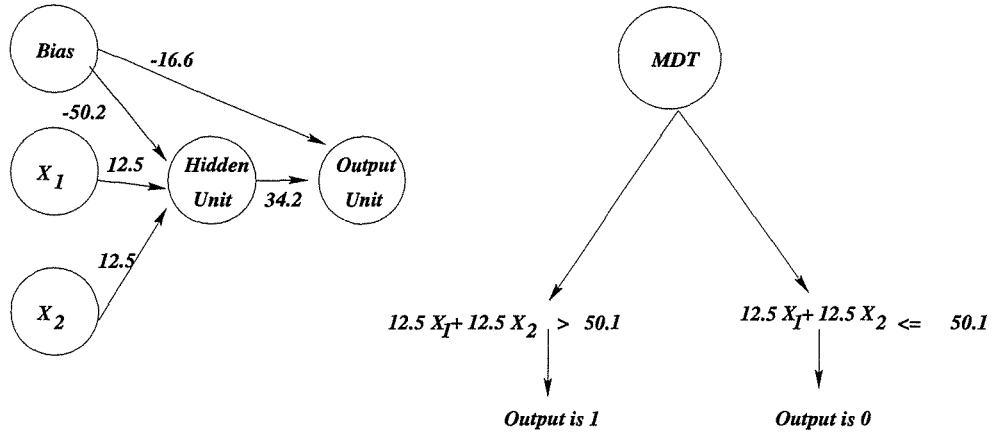

Figure 5.1: The ANN and the corresponding extracted MDT for a toy example representing a linear decision boundary using the function $x_1 + x_2 \leq 4$.

The two major contributions of this chapter are: an algorithm for generating MDTs by combining ANNs and UDTs, and the extension of decision trees with dynamic features; therefore opening new application domains for DTs.

5.2 Previous work in combining ANNs and DTs

In this section, previous work in integrating ANNs and DTs is presented. A number of studies have compared DTs and ANNs and motivated their integration. In a comparison between ID3 and ANNs, Brown et al. (1993) conclude that decision trees can be improved with multivariable splits and the performance of ANNs can be improved with feature selection. They further claim that decision trees can provide effective preprocessing for ANNs. Dietterich et al. (1995) compare ID3 with back-propagation on an English text-to-speech mapping problem and

find that ANNs capture statistical information whereas ID3 does not. They argue that the two methods' accuracy is comparable if ID3 is augmented with a simple statistical learning procedure.

One form of the integration is to grow an ANN as a DT using *Neural-trees*. Neural-trees are ANNs of restricted structure that can be easily interpreted as DTs. The Neural-tree algorithm (Sirat and Nadal 1990) is inspired by the tiling algorithm but with connections among neurons in the hidden layers disallowed. The resultant network can be visualised as a DT whose nodes correspond directly to hidden units. An improvement on Neural-trees, called *Trio-Learning*, was introduced by D'Alché-Buc et al. (1994) who utilised the fact that each intermediate node in the tree has two child nodes. Accordingly, training is carried out on a small tree consisting of a root node and its two child nodes. The results are slightly better than those of the Neural-Tree algorithm although at the expense of more extensive computations at each node.

Another way to integrate DTs and ANNs is to initialise the latter with the former in order to expedite and improve the convergence of ANN training. A version of ID3, called continuous ID3 (Cios and Liu 1992), converts UDTs into ANNs. Each level in the tree generated by ID3 is mapped to a hidden layer in the ANN being constructed but for large UDTs, the corresponding ANN architecture becomes impractical. In another attempt to speed up ANN training, Park (1994) introduced an algorithm for initialising an ANN with a linear tree classifier. The algorithm maps any linear tree classifier into an ANN with either one or two hidden layers. He has shown that every convex decision region enclosed by a subset of explicit hyperplanes of a tree, can be mapped to a neuron in the hidden layer. From my point of view, this is a very expensive process since the number of convex decision regions is exponential in the number of hyperplanes.

Finally, oblique rules have been generated from ANNs by Setiono and Huan (1995) who introduced a three-phase algorithm for extracting oblique rules from single hidden-layer ANNs. In the first phase, a network is trained with a weight decay term, and pruned in the second phase, with the activation values of hidden units discretised with a clustering algorithm in a third phase. The extraction process becomes easy after discretisation with rules effectively generated. The algorithm is computationally expensive at both the pruning and discretisation phases. As an enhancement, in a later paper (Setiono and Huan 1997) they re-present the training set to the

ANN after the training is completed, when outputs from the hidden units are discretised by a clustering algorithm using the statistical χ^2 test.

Maire (1999) introduced a general algorithm with a solid theoretical foundation, in terms of optimisation theory, for back projection of a set of polyhedra that define decision regions. He utilises a *threshold* selected by the user for the ANN, which determines whether the instance belongs to a positive or a negative class. This threshold is used as a constraint on the output unit and by back projection of this constraint through the network, polyhedra are determined. He proposes discretising the polyhedra after projecting back to the input layer. The main advantage is that this delayed discretisation guarantees high fidelity between the network and the resultant rules. The salient drawback of this algorithm, regardless of its generality and theoretical foundation, is the computational effort involved. For example, during the affine transformation phase in the algorithm, one of the steps requires the removal of redundant inequalities. Computationally, this is very expensive since for each inequality, a system of constraints should be solved to check whether or not the inequality is redundant. Even with fast algorithms for solving linear programming (Ami 1993) or employing sensitivity analysis, the computations involved are still expensive.

In summary, most of the integration between DTs and ANNs takes the form of growing ANNs as DTs and only a few studies concentrate on extracting oblique rules from ANNs. To my knowledge, none of the previous studies investigated the use of UDTs to generate MDTs from ANNs. Furthermore, integration efficiency is an outstanding issue and there remains the need for a simple, efficient algorithm for extracting oblique relations from an ANN which retains high fidelity with the network.

5.3 The C-net algorithm

The proposed algorithm, C-Net, has three stages and employs an ANN with a single hidden layer which is not a severe constraint since a neural network with a single hidden layer can approximate any arbitrary function to any degree of accuracy (Irie and Miyake 1988). There is no constraint on the type of the activation functions employed.

5.3.1 ANN training

The ANN can be trained with any training algorithm although we employed the stochastic gradient version of the back-propagation algorithm (*ie.* weights are updated after the presentation of each training pattern). The previously mentioned notations of ANN are adopted.

Following network training, training, validation, and test sets are re-introduced and the output of each hidden unit is calculated. Let $< X_{training}, Y_{training} >$, $< X_{validation}, Y_{validation} >$, and $< X_{testing}, Y_{testing} >$ denote the set of training, validation, and testing examples respectively, and the sets $< H_{training}, Y_{training} >$, $< H_{validation}, Y_{validation} >$, and $< H_{testing}, Y_{testing} >$ the corresponding Hidden-Output Mapping. Therefore, $H_{training}$ is the set of vectors generated by the hidden layer when presented with the training set $X_{training}$. The output layer is no longer required but retain the sets $< H_{training}, Y_{training} >$, $< H_{validation}, Y_{validation} >$, and $< H_{testing}, Y_{testing} >$ for the next stage of the algorithm.

5.3.2 Classification of the hidden to output mapping

The training set, $< H_{training}, Y_{training} >$, validation set, $< H_{validation}, Y_{validation} >$, and test set, $< H_{testing}, Y_{testing} >$, from the previous stage undergo classification using the gain ratio criterion of Quinlan (1993). This is the ratio of the gain resulting from splitting the data to the average amount of information required to identify the classes in the data. Suppose that the training set consists of n examples covering a space S with c classes. The entropy function $E(S)$ measures the degree of "impurity" in a collection of training examples, and is defined by $E(S) = \sum_{i=1}^{c} -p_i log_2 p_i$ where p_i is the relative frequency of class i in the space. The information gain, $G(S, A)$, measures the reduction in the expected entropy of the vectors of S caused by splitting on attribute A. Quinlan gives

$$G(S, A) = E(S) - \sum_{i \in \Phi(A)} \frac{|S_i|}{|S|} E(|S_i|) \tag{5.1}$$

where $\Phi(A)$ is the set of all possible values for attribute A, $|S_i|$ is the frequency of the value i for attribute A in the space, $E(|S_i|)$ measures the degree of "impurity" in a class i and equals

$-p_i log_2 p_i$, and we use $|S|$ to denote $\sum |S_i|$. However, this measure is biased toward attributes with many values (Mitchell 1997) since splitting on these attributes results in a higher value of the information gain because of the decrease in the number of instances in each subset. Subsequently, Quinlan adopted the gain ratio, $R = \frac{G}{T}$, where T is the information split criterion which measures how broadly and uniformly the attribute splits the data and is given by

$$T = -\sum_{j=1}^{c} \frac{|S_j|}{|S|} log_2 \frac{|S_j|}{|S|} \tag{5.2}$$

5.3.3 Back projection of decision trees

A DT is a disjunction of polyhedra where each polyhedron is a conjunction of linear constraints. In the resultant decision tree from the previous section, each constraint takes the form $H_j \leq RHS_j$, where RHS_j is a scalar specifying the split on that attribute and H_j is the output of hidden unit j as defined previously. To project back this axis-parallel hyperplane, the inverse of RHS_j is calculated viz $\sigma^{-1}(RHS_j)$ and H_j is replaced by the weighted sum of the corresponding input units, that is

$$\sum_{i=1}^{I} w_{ij} X_i \leq \sigma^{-1}(RHS_j) \tag{5.3}$$

It is obvious that projecting back an axis-parallel hyperplane is computationally less expensive than projecting back an oblique hyperplane as in (Maire 1999) since the former one generates two halfspaces while the latter results in a set of polyhedra. In our implementation, the activation function is taken to be the logistic function where the inverse is,

$$\sigma^{-1}(z) = -\frac{1}{D} ln(\frac{1-z}{z}), z \neq 0 \tag{5.4}$$

As an example, assume that one of the conditions on a node is $H_1 \leq 0.5$, where $H_1 = \sigma(3 \times X_1 - 4 \times X_2 + 3)$. Since $\sigma^{-1}(0.5) = 0$, the condition on the node will be $(3 \times X_1) - (4 \times X_2) \leq -3$ or equivalently $(-3 \times X_1) + (4 \times X_2) \geq 3$.

5.4 Experiments and comparisons

5.4.1 Methods and performance measures

The three stages in the algorithm are summarised in Figure 5.2 where we use C5, with standard parameters settings and without pruning, for discretising the hidden-output mapping. The activation function for the neural network is the sigmoid with a sharpness of 1.

- *Train a neural network with* $< X_{training}, Y_{training} >$, *until it reaches a satisfactory performance on* $< X_{validation}, Y_{validation} >$.
- *(1) Re-present* $< X_{training}, Y_{training} >$, $< X_{validation}, Y_{validation} >$, *and* $< X_{testing}, Y_{testing} >$ *to the trained network and store* $< H_{training}, Y_{training} >$, $< H_{validation}, Y_{validation} >$, *and* $< H_{testing}, Y_{testing} >$.
  (2) Train C5 with $< H_{training}, Y_{training} >$ *and* $< H_{validation}, Y_{validation} >$.
  (3) Test C5 with $< H_{testing}, Y_{testing} >$.
- *Replace each condition in the resultant UDT,* $(H_j \ op \ RHS_j)$, $op \in \{\leq, <, \geq, >, =\}$, *with* $(\sum_{i=1}^{I} w_{ij} X_i \ op \ \sigma^{-1}(RHS_j))$,

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Figure 5.2: The C-Net algorithm

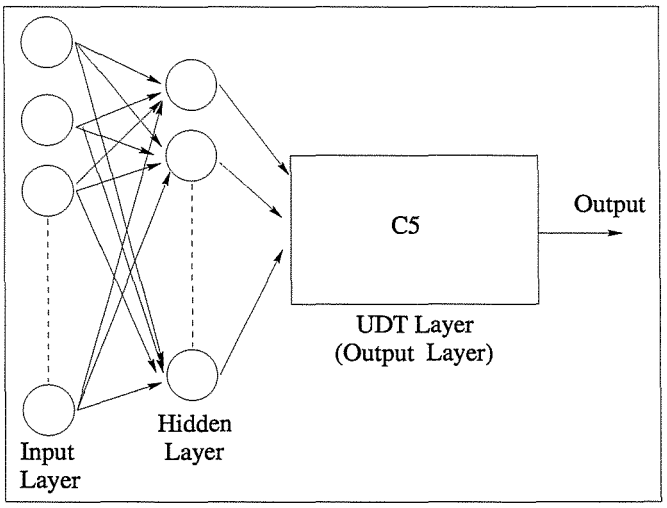

Figure 5.3: The C-Net conceptual representation.

To clarify this chapter's essential concepts, two types of comprehensibility are distinguished. The

first type, *expressiveness*, refers to the human brain's ability to understand the representational language of the classifier. The second, *compactness*, refers to the ability of representing a system with the minimum number of relations and symbols. Compactness is similar to the minimum description length principle (Quinlan and Rivest 1989) if we consider the message as the system and the string as a single relation to be transformed. It is clear that UDTs are more expressive than ANNs, since their representational language can easily be transferred into a set of "If ... Then" rules which are easily interpretable by the human brain. However, ANNs usually produce more accurate results than UDTs (Quinlan 1993) and they are also more compact.

Two performance measures have been used for the comparison between C5 and C-Net:

1. The percent bit error; that is, the percentage of misclassified cases on the test set. This measures the generalisation accuracy of the algorithm.

2. The tree size or the number of paths in the tree which is a measure of compactness and is equivalent to the number of paths (or leaves) in the DT (without pruning).

5.4.2 Data sets and experimental setup

Firstly, four real-life data sets were used to test C-Net. Three of these - Liver, Haberman, and Wisconsin Breast Cancer data sets - were down-loaded from the UCI repository of machine learning (Murphy and Aha 1992). The fourth data set is the dairy data. Each of the three UCI data sets were divided into a training, validation, and test sets consisting of 80%, 10%, and 10% of the data respectively (Quinlan 1993). The dairy data was divided into 25%, 25%, and 50% for training, validation, and testing respectively. Ten-fold cross-validation [1] was used while maintaining the class-distribution in the training, validation, and test sets. For the dairy data, the ten-fold were generated by sampling from the data at random without replacement. In Table 5.1, some statistics about the four data sets are summarised.

Secondly, the effectiveness of the C-Net algorithm on the following polynomials, which define the

[1] In cross-validation, the data is divided into ten subsets and the experiments are repeated ten times with each of these subsets as the test set and the other nine divided into one for validation and eight for training.

Table 5.1: Summaries of statistics for the real life databases

Database	Number of instances	Number of input attributes	The domain of each attribute
Breast Cancer	699	9	discrete values 1-10
Haberman	306	3	discrete values
Liver	345	6	continuous values
Dairy	25985	3	continuous values

decision boundary of the classification problem, are examined:

$$y = \begin{cases} 1, & if \quad x_1^n + x_2^n \geq 4, \\ 0, & if \quad x_1^n + x_2^n < 4. \end{cases} \tag{5.5}$$

for $n = 2, 3, 4$, or 5, forming the problems $P2, \ldots, P5$. Each variable, X_1 and X_2, is sampled from independent uniform distributions in the interval [0,5] subject to the constraint, $3 \leq x_1^n + x_2^n \leq 5$ so that the data are intensively sampled around the class boundary. A data set with 4000 points was generated for each model. Ten-fold cross-validation was adopted where the training, validation, and test sets contained 80%, 10%, and 10% of the data, respectively, while maintaining the class-distribution in the three sets.

For all problems, a learning rate of 0.03 and zero momentum were used for training four ANNs architectures with 2, 3, 4, and 5 hidden units. The networks for each of the 10-fold cross-validations were initialised with different weights, randomly drawn from independent uniform distributions in the range $[-0.1, 0.1]$. Each network ran for 10,000 epochs with validation performed after each epoch and the network with the smallest error on the validation set over all epochs was chosen.

After ANN training is completed the training, validation, and test sets were re-presented to the trained network, and the hidden output mapping was generated for subsequent presentation to C5 to generate the MDT.

5.4.3 Results and discussion

In Table 5.2, the performance of C-Net, C5, and ANN, on the eight data sets, is shown. The ANN, and its corresponding C-Net, shown in the table is the one whose number of hidden units

achieved the best generalisation during the experiments. On the four real-life problems, the bit-error of C-Net is less than the corresponding bit error of ANN which C-Net was extracted from. This improvement ranged from 0.1% to 12%. Also, C-Net always generalises better than C5 where in some cases is 45% more accurate than C5. In terms of the size of the trees generated by C-Net and C5, C-Net always resulted in smaller trees. The reduction in the tree-size ranged, on the average, from 62% for the four real-life problems to 31% for the four artificial data sets. However, one should bear in mind that the computations at each node increased in MDTs.

Table 5.2: The average percentage bit error of C-Net, C5, and ANN on the test set for the eight data sets.

Problem	C-Net	C5	ANN
Breast Cancer	$2.2\% \pm 1.6^{\dagger}$	$4.9\% \pm 2.3$	$2.5\% \pm 1.8$
	2.0 ± 0.5	20.3 ± 1.0	2
Haberman	$28.4\% \pm 2.3$	$28.8\% \pm 4.6$	$28.8\% \pm 4.6$
	3.3 ± 0.6	4.0 ± 1.6	2
Liver	$31.7\% \pm 7.8^{\ddagger}$	$37.4\% \pm 5.5$	$32.6\% \pm 7.9$
	7.5 ± 3.0	21.5 ± 5.7	5
Dairy	$22.7\% \pm 0.4$	$22.9\% \pm 0.4$	$23.3\% \pm 1.4$
	2.0 ± 0.0	8.4 ± 3.5	2
P2	$2.3\% \pm 1.2$	$2.7\% \pm 1.1$	$1.4\% \pm 1.2$
	30.3 ± 6.7	53.8 ± 4.0	4
P3	$1.7\% \pm 0.4^{\oplus}$	$2.4\% \pm 0.8$	$0.5\% \pm 0.6$
	31.1 ± 5.0	40.2 ± 1.4	5
P4	$1.4\% \pm 0.8^{\ddagger}$	$2.6\% \pm 0.6$	$0.6\% \pm 0.7$
	30.6 ± 2.0	47.6 ± 3.5	5
P5	$2.6\% \pm 1.2^{\oplus}$	$3.4\% \pm 1.0$	$0.8\% \pm 0.6$
	34.1 ± 12.6	40.0 ± 2.2	5

For each problem, the upper row gives the average percentage bit error for C-Net, C5, and the corresponding ANN from which C-Net was extracted. The lower line for each problem gives the number of leaves in the tree computed by C-Net (column 2) and C5 (column 3), and the number of hidden units for the best ANN which C-Net was extracted from. Rows labeled †, ‡, and ⊕, indicate that C-Net results are significantly different from C5 at $\alpha = 0.0005, 0.005$, and 0.01, respectively.

It is to be expected that C-Net is less accurate than ANN since C-Net's piecewise linear approximation is expected to lose the smoothness of the original continuous nonlinear function represented by the ANN. However, C-Net generalised better than the corresponding ANN on the four real-life problems (Table 5.2). For the four artificial data sets, ANN generalised better than C-Net because the data were generated around the decision boundaries; therefore, C-Net's

approximation of the nonlinear function generated by ANN becomes harder.

In comparing C-Net with C5, we can see from Table 5.2 (columns 2 and 3, the first row in each problem) that C-Net generalises better than C5 since it results in the smallest error on the test set and also a very small tree size in most cases. Nevertheless, one should bear in mind that the representational language (expressiveness) of the trees produced by C-Net is less expressive (less comprehensible to the human mind) than that produced by C5.

The dependence of the performance of C-Net on the number of hidden units used in the corresponding ANNs is examined. The size of the tree generated by C-Net is compared with the number of hidden units in each problem. Table 5.3 shows the C-Net tree-size for each network architecture. It can be seen from the table that, in the four real-world problems, the size of the DT generated by C-Net is small. Also, it varies little across network architectures, indicating that C-Net performance is not so sensitive to the architecture of its component ANN. For the four artificial data sets, although the size of C-Net does not vary much across different hidden units, it is quite large for the four artificial data sets. The reason for this is obvious since C-Net requires more hyperplanes to approximate the underlying non-linear function.

Table 5.3: The average tree-size of C-Net on each architecture for the eight data sets.

Problem	Number of Hidden Units			
	2	**3**	**4**	**5**
Breast Cancer	**2.0±0.5**	3.6±2.1	3.8±1.9	3.2±1.7
Haberman	**3.3±0.6**	3.0±0.0	2.9±0.4	3.4±1.5
Liver	3.5±1.1	4.6±2.9	5.0±2.4	**7.5±3.0**
Dairy	**3.0±1.5**	3.4±1.8	3.6±2.0	4.9±3.7
P2	35.1 ± 3.7	34.9 ± 3.2	**30.3 ± 6.7**	23.7 ± 5.4
P3	29.8 ± 1.7	40.3 ± 2.9	37.6 ± 7.6	**31.1 ± 5.0**
P4	37.2 ± 2.8	49.2 ± 4.1	39.5 ± 12.3	**30.6 ± 2.0**
P5	32.9 ± 2.5	42.6 ± 8.8	43.0 ± 11.4	**34.1 ± 12.6**

The tree-sizes are the average over ten-fold cross-validation with different weight initialisation ± the standard deviation. Bold faces indicate the best result found in Table 5.2.

5.5 Recurrent C-Net

In this section, C-Net is used in the context of a new kind of decision tree, that is a *recurrent decision tree* (RDT). DTs are limited since they lack any recurrent capabilities. However, if a *simple recurrent neural network* (SRN) is substituted for the feedforward one in Figure 5.3, the resultant DTs can be assisted to incorporate recurrent features. After training the SRN, the recursive function thereby generated by the network may be interpreted as an easy to understand RDT. The required algorithm is similar to that described in Section 5.3 except for the concept of projecting the tree back through the neural network. We introduce the following dynamics to replace Equation 6.3.

$$\sum_{i=1}^{I} w_{ij} X_i(t) + \sum_{c=1}^{J} w_{cj} H_c(t-1) \leq \sigma^{-1}(RHS_j) \tag{5.6}$$

$$H_c(t) = \sigma(\sum_{i=1}^{I} w_{ij} X_i(t) + \sum_{c=1}^{J} w_{cj} H_c(t-1)) \tag{5.7}$$

$$H_c(0) = \sigma(\sum_{i=1}^{I} w_{ij} X_i(0)) \tag{5.8}$$

$H_c(t)$ is a sigmoid function equivalent to the values of the context unit of the SRN at time t. That is, the condition represented by Equation 5.6 at each node of the decision tree is a recursive function so that, each node effectively has a memory corresponding to Equations 5.7 and 5.8. This RDT has a lot of potential in many fields such as the possibility of mapping an SRN into its corresponding finite state automaton.

In the remainder of this section, the recurrent C-Net approach[2] is illustrated using an Elman-type SRN that has been trained on temporal sequences from a natural language data set (Towsey et al. 1998). The data set consists of strings of part-of-speech (POS) tags derived from natural language sentences obtained from a first year school reader. Each word in a sentence is replaced by its POS classification (ie. verb, noun, adverb etc). The SRN is required to predict the next POS given the current and previous context. Standard decision trees cannot perform this task because they lack the memory to store previous context. Therefore, the only comparison we are

[2]This experiment was performed by Dr. Michael Towsey

making is between the performance of C-Net and the standard Elman SRN.

When applying the Elman SRN to the natural language data, error on the test set decreased from 44.8% to 31.4% as the number of hidden units was increased from 2 to 8 (Table 5.4). The test error of C-Net also tended to decrease as the number of hidden units increased but less steeply. Consequently, C-Net performed better than the SRN for 2, 3 and 4 hidden units but worse when 8 or more hidden units was used. The optimum number of hidden units for C-net was 4 and for SRN was 8. These results suggest that with a small number of hidden units, the output layer of the SRN is unable to capture all the information encoded in the outputs from the hidden units, whereas C5 is better in this respect. However once the number of hidden units is 8 or more for this problem, the SRN output layer is better suited than C5 to learning the hidden unit representation.

Table 5.4: Performance of recurrent C-Net on a natural language data set.

Problem	Number of Hidden Units				
	2	**3**	**4**	**6**	**8**
SRN % Bit error	44.8% ± 2.9	40.9% ± 2.5	**37.6% ± 1.9**	33.4% ± 1.8	31.4% ± 1.5
C-Net % Bit error	36.5% ± 3.6	33.9% ± 1.4	**33.1% ± 2.1**	33.4% ± 1.7	34.4% ± 1.7
C-Net Tree size	29.1 ± 6.3	37.7 ± 7.3	**44.2 ± 12.0**	49.9 ± 12.1	56.8 ± 7.5

Percent bit error obtained by SRN and C-Net on a test set of natural language data for SRNs having different numbers of hidden units and the size of the tree generated in each case. Averages and standard deviations are for 10 repeats of SRN initialised with different initial weights. For all hidden unit numbers (except 6 hidden units), the difference between SRN error and C-Net is significant at confidence level 0.001.

5.6 Conclusion

In this chapter, a novel algorithm, C-Net, is introduced for generating multivariate decision trees from artificial neural networks using a univariate decision tree, C5. The resultant tree, when compared with the tree generated by C5 alone, is more compact and accurate. Furthermore, it is more expressive than the corresponding artificial neural network. We believe that using a hybrid system which combines C5, as one of the strongest decision tree classifiers, and the multi-layer

feedforward ANN, as a strong non-parametric nonlinear regression model, results in a hybrid method that is an enhancement for both technologies. Although for our problems, C-Net was always more accurate than C5, it is not conclusive that this is the universal case. Rather, methods are more or less more suitable for specific domains. Our conclusion is that the integration of decision trees and artificial neural networks is a necessity if the application domain requires accurate, compact, and expressive predictive ability, in which case, C-Net can play a significant role.

Additionally, C5 employs the statistical χ^2 test for deciding when to cease training. This is found to be robust against the number of hidden units used for the ANN. This point is illustrated when the size of the trees generated by C-Net was almost identical regardless of the number of hidden units in some cases (for example Haberman). This indicates that the addition of more hidden units in some cases was not required and can be used as an indication of redundancies in the ANN's architecture.

Furthermore, C-Net can be used to generate recurrent decision trees where a memory is associated with each node in the tree and the conventional linear condition attached to each node is replaced by a recursive function. The potential of recurrent decision trees is enormous and it opens a new area of application to conventional DTs.

C-Net looks promising since it has the advantage of conventional ANNs, that, with their piecewise linear approximation, they are expected to be more accurate than UDTs. Also, it has the advantage of UDTs, that their representational language is more expressive than ANNs. Furthermore, it combines the two technologies, UDTs and ANNs, in a frame that is easy to implement and balances between compactness, expressiveness, and accuracy better than any of these technologies in isolation.

In the previous chapter, we experimented with both ANNs and DTs. This motivated the idea of C-Net. The current chapter presented still some results regarding the prediction problem; therefore emphasizing the second thesis sub-objective; discovering patterns in the dairy database using KDD. The rest of the thesis will discuss the third thesis sub-objectives; that is, formulating and solving the mate-selection problem.

Part III

Optimisation Models

Chapter 6

Heuristics for Complex Optimisation Problems

This chapter's main objective is to introduce the foundations of the techniques to be used for solving the mate-selection problem in the following chapters. A general introduction is given in Section 6.1 and seven heuristic search techniques are then presented. More specifically, *simulated annealing* (SA) is presented in Section 6.2 followed by *tabu search* (TS) in Section 6.3, *genetic algorithm* (GA) in Section 6.4, *differential evolution* (DE) in Section 6.5, *immune systems* in Section 6.6, *ant colony optimisation* (ACO) in Section 6.7, and *memetic algorithms* (MA) in Section 6.8. Issues arising with constraints and multi-objectives are discussed in Sections 6.9 and 6.10, respectively.

6.1 Introduction

Optimisation theory provides a compact set of techniques to handle different types of optimisation problems. Unfortunately, real life problems are known to be messy, complex, multi-objective, dynamic, uncertain, and large scale; that is, the problem has large numbers of variables and constraints. Conventional optimisation techniques cannot handle these complex problems in a reasonable time. Heuristic search techniques provide a means for handling these complex problems at the cost of returning a near, in contrast to an exact, optimal solution. There used to be a distinction between conventional optimisation techniques and heuristics but this is becoming increasingly less clear because there is much in common between the two.

The general optimisation problem (hereafter referred to as P1) can be stated as:-

$$\text{(P1): Minimise } f(x)$$
$$\text{subject to: } M = \{x \in R^n | G(x) \leq 0\}$$

where x is the set of decision variables, $f(x)$ is the objective function, $G(x)$ is a set of constraints, and M is the set of feasible solutions. If the optimisation problem is maximisation, it is equivalent to a minimisation problem after multiplying the objective by (-1). Also, if a constraint is an equation, it can be represented by two inequalities one is "less than or equal" while the other is "greater than or equal". A "greater than or equal" inequality can be transformed to a "less than or equal" inequality by multiplying both sides by (-1). In summary, any optimisation problem can be represented in the previous general form.

Let us define three sets, $M_1 = \{x \in R^n | x_j \text{ is integer}, j = 1 \ldots n\}$, $M_2 = \{x \in R^n | x_j \text{ is integer}, j \in J \subset \{1 \ldots n\}\}$, and $M_3 = \{x \in R^n | x_j \in \{0, 1\}, j = 1 \ldots n\}$. Three special cases from the general optimisation problem - the pure integer, mixed integer, and binary optimisation problems - can be defined respectively as follows:

$$\text{(P2): Minimise } f(x)$$
$$\text{subject to: } M \cap M_1$$

$$\text{(P3): Minimise } f(x)$$
$$\text{subject to: } M \cap M_2$$

$$\text{(P4): Minimise } f(x)$$
$$\text{subject to: } M \cap M_3$$

Hereafter, $\theta(x)$ will be used generically to represent the feasible region of any optimisation problem. For example, $\theta(x)$ is M in P1, $M \cap M_1$ in P2, $M \cap M_2$ in P3, and $M \cap M_3$ in P4.

Two important types of optimal solutions will be referred to in the rest of this thesis, local and global optimal solutions. Let us define the open ball (*ie.* a neighbourhood centred on $\bar{x}$ and defined by the Euclidean distance) $B_\delta(\bar{x}) = \{x \in R^n | \ ||x - \bar{x}|| < \delta\}$.

Definition 1: Local optimality A point $\bar{x} \in \theta(x)$ is said to be a local minimum of the optimisation problem iff $\exists\ \delta > 0\ \ni\ f(\bar{x}) \leq f(x), \forall x \in (B_\delta(\bar{x}) \cap \theta(x))$.

Definition 2: Global optimality A point $\bar{x} \in \theta(x)$ is said to be a global minimum of the optimisation problem iff $f(\bar{x}) \leq f(x), \forall x \in \theta(x)$.

Usually, there is more than a single objective to be optimised in real life applications. In this case, the problem is called *multi-objective vector optimisation problem* (VOP). Each of the four problems, P1 to P4, can be re-defined as general multi-objective problems, VOP1 to VOP4 respectively, by replacing the objective function $f(x)$ with a vector of objectives $F(x)$. For example, the multi-objective version of P1 is VOP1 as follows:

$$\text{(VOP1): Minimise } F(x)$$
$$\text{subject to: } M = \{x \in R^n | G(x) \leq 0\}$$

In a problem with conflicting objectives, the existence of a unique optimal solution is no longer a valid concept. The solution which satisfies the optimality conditions of one objective may be a bad solution for another. Consequently, we need to redefine the concepts of local and global optimality in multi-objective problems. To do this, we define two operators, $\gneqq$ and $\precnsim$ and then assume two vectors, X and Y. $X \gneqq Y$ iff $\exists\ x_i \in X$ and $y_i \in Y\ \ni\ x_i \neq y_i$. $X \precnsim Y$ iff $\forall\ x_i \in X$ and $y_i \in Y, x_i \leq y_i$, and $X \gneqq Y$. $\gneqq$ and $\precnsim$ can be seen as the "not equal to" and "less than or equal to" operators over two vectors. We can now define the equivalent concepts of local and global optimality in VOP.

Definition 3: Local efficient (non-inferior/pareto-optimal) solution A point $\bar{x} \in \theta(x)$ is said to be a local efficient solution of VOP iff $\nexists\ x \in (B_\delta(\bar{x}) \cap \theta(x))\ \ni\ F(x) \precnsim F(\bar{x})$ for some positive δ.

Definition 4: Global efficient (non-inferior/pareto-optimal) solution A point $\bar{x} \in \theta(x)$ is said to be a global efficient solution of VOP iff $\nexists\ x \in \theta(x)\ \ni\ F(x) \precnsim F(\bar{x})$.

Definition 5: Non-dominated solution A point $\bar{y} \in F(\bar{x})$ is said to be non-dominated solution of VOP iff $\bar{x}$ is an efficient solution of VOP.

Optimisation theory provides strong foundations for solving different types of optimisation problems. Unfortunately, all methods introduced by optimisation theory have an assumption or more;

least of which is that they are specific to a particular model. This lack of a general algorithm which does not have pre-assumptions about the model, causes optimisation theory to fail in front of some complex real life problems. However, if an optimisation method is suitable for a specific model, it guarantees optimality if it exists (although not necessarily global optimality). By contrast, heuristic algorithms provide a means for solving general optimisation problems at the cost of returning a near optimal solution. If the problem for optimisation is in formulating the model so that it closely resembles reality without violating the assumptions of the technique (for example, convexity assumption), the problem for heuristic algorithms is in determining an appropriate value for the search parameter(s) in each problem.

Before proceeding with the rest of this chapter, it is important to first introduce some basic terminologies in complexity theory that we will use in later chapters, and also introduce *multi-stage decision models*, which is the formulation approach used in later chapters. The following definition is extracted from (Ansari and Hou 1997).

> Suppose f and g are positive functions defined for positive integers, $f,\ g\ :\ I^+ \rightarrow R^+$, and Q and $Prob$ are two problems, then
>
> 1. $f = O(g)$, if $\exists$ positive constants c and N such that $f(n) \leq cg(n)$, $\forall\ n \geq N$.
> 2. If $Prob$ can be solved in a polynomial time and $\exists$ a polynomial time algorithm L where L can transform Q to $Prob$ (ie. polynomial time reduction), then $\exists$ a polynomial time algorithm to solve Q.
> 3. A particular class of decision problems that can be solved in polynomial time by a nondeterministic computer is known as NP.

Multi-stage decision modeling is a modeling approach rather than a solution mechanism (eg. *linear programming*). Thus, it is an art for decomposing large scale problems in terms of stages linked with a set of transitions. The model can be solved afterward with *dynamic programming* (Bellman and Dreyfus 1962) or other mathematical programming techniques. Sniedovich (1992) defines a multi-stage decision model as:

> "A collection (N, S, D, T, S_1, g) where

1. N is a positive integer specifying the number of *decision stages* comprising the decision-making process. Define $\mathcal{N} = 1, 2, 3, \ldots, N$. Thus, for $N = \infty$ the set $\mathcal{N}$ denotes the set of positive integers.

2. S is a non-empty set entitled the *state space*. Its elements are called *states*.

3. D is a function that to each pair $(n, s) \in \mathcal{N} \times S$, it assigns a subset of some set $\mathcal{D}$. The set $D(n, s)$ is referred to as the *set of feasible decisions* pertaining to state s at stage n. If the set $D(n, s)$ is empty, the state s is considered to be non-feasible at stage n. The set $\mathcal{D}$ is named the *decision space*.

4. T is a function on $\mathcal{N} \times S \times \mathcal{D}$ with values in S called the *transition function*. For any triplet (n, s, x) such that $n \in \mathcal{N}$, $s \in S$, and $x \in D(n, s)$, the element $s = T(n, s, x)$ designates the states at stage $n + 1$ resulting from the decision x application to the state s at stage n.

5. S_1 is a non-empty subset of S whose elements are named *initial states*.

6. g is a real-valued function on $S_1 \times \mathcal{D}^N$ termed the *objective function*. The value yielded by $g(s, x_1, x_2, \ldots, x_N)$ is understood to specify the overall cost or benefit arising from the decisions $(x_1, \ldots, x_N)$ made at stages $1, 2, 3, \ldots, N$ respectively, given that the initial process state is $s \in S_1$."

In this chapter, seven heuristic search techniques are introduced: SA, TS, GA, DE, Immune, ACO, and MA. Whether we are using conventional optimisation or heuristic methods to solve a general optimisation problem, two issues usually arise: how to handle the constraints, and how to solve the VOP. These two issues are discussed at the end of the chapter.

6.2 Simulated annealing

In the process of physical annealing (Rodrigues and Anjo 1993), a solid is heated until all particles randomly arrange themselves in the liquid state. A slow cooling is then used to crystallise the liquid. That is, the particles are free to move at high temperature and gradually lose their mobility by decreasing the temperature (Ansari and Hou 1997). This process is described by the early work in statistical mechanics of Metropolis (Metropolis et al. 1953) and is well-known as

the Metropolis algorithm, Figure 6.1.

Define the transition of the substance from state i with energy $E(i)$ to state j with energy $E(j)$ at temperature level T
If $E(i) \leq E(j)$ **then** *accept* $i \rightarrow j$
If $E(i) > E(j)$ **then** *accept* $i \rightarrow j$ *with probability* $exp(\frac{E(i)-E(j)}{KT})$ *where K is the Boltzmann constant*

Figure 6.1: Metropolis algorithm

Kirkpatrick et. al. (1983) defined an analogy between the Metropolis algorithm and the search for solutions in complex combinatorial optimisation problems where he developed the idea of SA. Simply speaking, SA is a stochastic computational technique that searches for global optimal solutions in optimisation problems. In complex combinatorial optimisation problems, it is usually easy to be trapped in a local optimum. The main goal here is to give the algorithm more time in the search space exploration by accepting moves, which may degrade the solution quality, with some probability depending on a parameter called the "*temperature*". When the temperature is high, the algorithm behaves like random search. A cooling mechanism is used to gradually reduce the temperature and the algorithm performs similar to a greedy hill-climbing algorithm when the temperature is frozen to zero. If this process is given sufficient time, there is a high probability that it will result in a global optimal solution (Ansari and Hou 1997). The algorithm escapes a local optimal solution by moving with some probability to those solutions which degrade the current one and accordingly gives a high opportunity to explore more of the search space. The probability of accepting a bad solution, $\pi(T)$, follows a Boltzmann (also known as Gibbs) distribution of:

$$\pi(T) = exp\left(\frac{E(i) - E(j)}{KT}\right) \tag{6.1}$$

where $E(i)$ is the energy or objective value of the current solution, $E(j)$ is the previous solution's energy, T is the temperature and K is a Boltzmann constant. In actual implementation, K can be taken as a scaling factor to keep the temperature between 0-1, if it is desirable that the temperature falls within this interval. Unlike GA, there is a proof for the convergence of SA (Ansari and Hou 1997) assuming that the time spent at each temperature level is sufficient.

The algorithm

There are two main approaches in SA: homogeneous and non-homogeneous (Vidal 1993). In the former, the temperature is not updated after each step in the search space, although for the latter it does. It is found that in homogeneous SA, the transitions or generations of solutions for each temperature level represent a Markov chain of length equal to the number of transitions at that temperature level. The homogeneous and non-homogeneous algorithms are shown in Figures 6.2 and 6.3 respectively.

The homogeneous algorithm starts with three inputs from the user, the initial temperature T, the initial Markov chain length L, and the neighbourhood length ζ. Then, it generates an initial solution, evaluates it, and stores it as the best solution found so far. After that, for each temperature level, a new solution is generated from the current solution neighbourhood $N(x', \zeta)$ (refer to Section 9.3.2 for our definition of a neighbourhood), tested, and replaces the current optimal if it is better than it. The new solution is then tested against the previous solution, if it is better, the algorithm accepts it; otherwise it is accepted with a certain probability as specified previously. After completing each Markov chain of length L, the temperature and the Markov chain length are decreased. The question now is: how to update the temperature T or the cooling schedule.

Cooling schedule

In the beginning of the simulated annealing run, we need to find a reasonable value of T such that most transitions are accepted. This value can be easily found through a small amount of experimentation. We then increase T with some factor until all transitions are accepted. Another way to do it is to generate a set of random solutions and find the minimum temperature T that guarantees the acceptance of these solutions. Following the determination of T, we need to define a cooling schedule for it. Two methods are usually used in the literature. The first is static, where we need to define a discount parameter α. After the completion of each Markov chain, k, adjust T as follows (Vidal 1993):

$$T_{k+1} = \alpha \times T_k, 0 < \alpha < 1 \tag{6.2}$$

initialise the temperature to T
initialise the chain length to L
initialise the neighbourhood length ζ
$x_0 \in \theta(x)$, $f_0 = f(x_0)$
initialise optimal solution x_{opt} *to be* x_0 *and its objective value* $f_{opt} = f_0$
initialise current solution x' *to be* x_0 *and its objective value* $f' = f_0$
repeat
  for $j = 0$ *to* L
    $i = i + 1$
    $x_i \in N(x', \zeta)$, $f_i = f(x_i)$
    $\Delta(f) = f_i - f'$
    if $f_i < f_{opt}$ **then** $x_{opt} = x_i$, $f_{opt} = f_i$
    if $f_i < f'$ **then** $x' = x_i$, $f' = f_i$
    else if $exp(-\Delta(f)/T) >$ *random (0,1)* **then** $x' = x_i$, $f' = f_i$
  next j
  update L *and* T
until *loop condition is satisfied*
return x_{opt} *and* f_{opt}

Figure 6.2: General homogeneous simulated annealing algorithm.

initialise the temperature to T
initialise the number of iterations to L
initialise the neighbourhood length ζ
$x_0 \in \theta(x)$, $f_0 = f(x_0)$
initialise optimal solution x_{opt} *to be* x_0 *and its objective value* $f_{opt} = f_0$
initialise current solution x' *to be* x_0 *and its objective value* $f' = f_0$
for $i = 0$ *to* L
  $x_i \in N(x', \zeta)$, $f_i = f(x_i)$
  $\Delta(f) = f_i - f'$
  if $f_i < f_{opt}$ **then** $x_{opt} = x_i$, $f_{opt} = f_i$
  if $f_i < f'$ **then** $x' = x_i$ *and* $f' = f_i$
  else if $exp(-\Delta(f)/T) >$ *random (0,1)* **then** $x' = x_i$, $f' = f_i$
  update T
next i
return x_{opt} *and* f_{opt}

Figure 6.3: General non-homogeneous simulated annealing algorithm.

The second is dynamic, where one of its versions was introduced by Huang, Romeo, and Sangiovanni-Vincetilli, 1986. Here,

$$T_{k+1} = T_k e^{-\left(\frac{T_k \Delta(E)}{\sigma^2_{T_k}}\right)} \tag{6.3}$$

$$\Delta(E) = E(T_k) - E(T_{k-1}) \tag{6.4}$$

where $\sigma^2_{T_k}$ is the variance of the accepted solutions at temperature level T_k.

6.3 Tabu search

Glover (1989, 1990) introduced *tabu search* (TS) as a method for escaping from a local optimum. The goal is to obtain a list of forbidden (tabu) solutions/directions in the neighbourhood of a solution to avoid cycling between solutions while allowing a direction which may degrade the solution although it may help in escaping from the local optimum. Similar to SA, we need to specify how to generate solutions in the current solution's neighbourhood. Furthermore, the temperature parameter in SA is replaced with a list of forbidden solutions/directions updated after each step. When generating a solution in the neighbourhood, this solution should not be in any of the directions listed in the tabu-list, although a direction in the tabu-list may be chosen with some probability if it results in a solution which is better than the current one. In essence, the tabu-list aims to constrain or limit the search scope in the neighbourhood while still having a chance to select one of these directions.

The algorithm

initialise the neighbourhood length to ζ
$x_0 \in \theta$, $f_0 = f(x_0)$.
$x_{opt} = x_0$, $f_{opt} = f_0$
$x' = x_0$, $f' = f_0$, $k = 1$
while *the stopping condition is not met* **do**
    $k = k + 1$
    choose $x_k \in N(x', \zeta)$
    if $f(x_k) < f(x_{opt})$ **then** $x_{opt} = x_k$, $f_{opt} = f_k$
    if $f(x_k) < f(x')$ **then** $x' = x_k$, $f' = f_k$
    else if $x_k \notin M$ **then** $x' = x_k$, $f' = f_k$
    update M *with* x_k
end while

Figure 6.4: The Tabu search algorithm

The TS algorithm is presented in Figure 6.4. A new solution x_k is generated within the current solution's neighbourhood $N(x', \zeta)$[1]. If the new solution is better than the optimal solution, it is accepted and saved as the optimal. If the new solution is better than the current solution, it is accepted and saved as the current solution. If the new solution is not better than the current

[1]The neighbourhood, as used in our implementation, will be defined in Section 9.3.2.

solution and it is not in a direction within the tabu list M, it is accepted as the current solution and the search continues from there. If the solution is tabu, the current solution remains the same. After accepting a solution, M is updated to forbid returning to this solution again. The function *choose* can be implemented in many different ways (refer to Section 9.9 for our implementation of this function).

The list M can be a list of the tabu solutions visited in the last n iterations. However, this is a memory consuming process and it is a limited type of memory. Another possibility is to define the neighbourhood in terms of a set of moves. Therefore, instead of storing the solution, the reverse of the move which produced this solution is stored instead. Clearly, this approach prohibits, not only returning to where we came from, but also many other possible solutions. Notwithstanding, since the tabu list is a short term memory, at some point in the search, the reverse of the move will be eliminated from the tabu list, therefore, allowing to explore this part of the search space which was tabu.

A very important parameter here, in addition to the neighbourhood length which is a critical parameter for many other heuristics such as SA, is the choice of the tabu-list size which is referred in the literature as the method's *adaptive memory*. This is a problem-dependent parameter, since the choice of large size would be inefficient in terms of memory capacity and the time required to scan the list. On the other hand, choosing the list size to be small would result in a cycling problem; that is, revisiting the same state again (Glover 1989). In general, the tabu-list's size is a very critical issue for the following reasons:-

1. The performance of tabu search is sensitive to the size of the tabu-list in many cases.

2. There is no general algorithm to determine the optimal tabu-list size apart from experimental results.

3. Choosing a large tabu-list is inefficient in terms of speed and memory.

6.4 Genetic algorithm

In trying to understand evolutionary mechanisms, Holland (1998) devised a new search mechanism, which he called genetic algorithm, based on Darwin's (1859) principle of natural selection. In its simple form, genetic algorithm recursively applies the concepts of *selection*, *crossover*, and *mutation* to a randomly generated population of promising solutions with the best solution found being reported. A generic GA algorithm is presented in Figure 6.5. GA is contingent upon coding the parameters. Therefore, the choice of the right representation is a crucial issue (Goldberg 1989). In its early stage, Holland (1998) coded the strings in GA using the binary set of alphabets {0,1}, that is binary representation. He introduced the *Schema Theorem*, which provides a lower bound on the change in the sampling rate for a single hyperplane from one generation to another. A schema is a subset of the solution space whose elements are identical in particular loci. It is a building block that samples one or more hyperplanes. Other representations use integer or real numbers.

let G denote a generation, P a population, and x^l the lth chromosome in P
initialise the initial population of M solutions $P_{G=0} = \{x^1_{G=0}, \ldots, x^M_{G=0}\}$
evaluate every $x^l \in P_{G=0}$, $l = 1, \ldots, M$
k=1
while *the stopping criteria is not satisfied* **do**
    select P' (an intermediate population) from $P_{G=k-1}$
    $P_{G=k} \leftarrow$ crossover elements in P'
    mutate elements in $P_{G=k}$
    evaluate every $x^l \in P_{G=k}$, $l = 1, \ldots, M$
    $k = k + 1$
return *$x = arg\max_l f(x^l), x^l \in P_{G=k}$, the best encountered solution*

Figure 6.5: A generic genetic algorithm

The algorithm

Selection

As with animal breeding, there are many alternatives for selection in GA. One method is based on the principle of "living for the fittest" or *fitness-proportionate selection*, (Jong 1975), where the objective functions' values for all the population's individuals are scaled and an individual

is selected in proportion to its fitness. The fitness of an individual is the scaled objective value of that individual. The objective values can be scaled in differing ways. Let us define Obj_l and $Fitness_l$ to be the objective and fitness values of chromosome l respectively. Let the population size be M. *Roulette wheel selection* is a fitness-proportionate selection where the scaled fitness is

$$Fitness_l = \frac{Obj_l}{\sum_{j=1}^{M} Obj_j} \tag{6.5}$$

Each individual is then assigned a slot on a roulette wheel equivalent to its fitness. Every time the wheel spins, the imaginary ball (random number) falls in one of the slots and the corresponding individual is selected. Other types of scaling are *window-scaling*:

$$Fitness_l = \frac{Obj_l \ - \ \min_j(Obj)}{\max_j(Obj) \ - \ \min_j(Obj)} \tag{6.6}$$

and *sigma-scaling*:

$$Fitness_l = \frac{Obj_l \ - \ \frac{\sum_{j=1}^{M} Obj_j}{M}}{\sigma(Obj)} \tag{6.7}$$

Another way to adopt the fitness-proportionate selection is to use *rank-based selection* where all individuals in the population are ranked according to their objective values, and selection is carried out in proportion to the rank.

Another alternative is *stochastic-Baker selection* (Goldberg 1989), where the objective values of all the individuals in the population are divided by the average to calculate the fitness, and the individual is copied into the intermediate population a number of times equal to the integer part, if any, of the fitness value. The population is then sorted according to the fraction part of the fitness, and the intermediate population is completed with a fitness-proportionate selection.

Tournament selection is another famous strategy (Wetzel 1983), where N chromosomes are chosen uniformly irrespective of their fitness and the fittest of these is placed into the intermediate population. As this is usually expensive, a modified version called *modified tournament selection* (Ross 1996) works by selecting an individual at random and up to N trials are made to pick a fitter one. The first fitter individual encountered is selected; otherwise, the first individual wins.

Reproduction strategies

A reproduction strategy is the process of building a population of individuals in a generation from a previous generation. There are a number of reproduction strategies presented in the literature, among them, *canonical*, *simple*, and *breedN*. Canonical GA (Whitley 1994) is similar to Schwefel's (1981) evolutionary strategy where the offspring replace all the parents; that is, the crossover probability is 1. In simple GA (Ross 1996), two individuals are selected and the crossover occurs with a certain probability. If the crossover takes place, the offspring are placed in the new population; otherwise the parents are cloned. *Breeder Genetic Algorithm* (Mühlenbein and Schlierkamp-Voosen 1993; Mühlenbein and Schlierkamp-Voosen 1994) or the breedN strategy is based on quantitative genetics. It assumes that there is an imaginary breeder who performs selection of the best N strings in a population and breed among them. Mühlenbein (1994) comments that if "GA is based on natural selection", "breeder GA is based on artificial selection".

Another popular reproduction strategy, *parallel genetic algorithm* (Mühlenbein et al. 1988; Mühlenbein 1991), employs parallelism. In parallel GA, a number of populations evolve in parallel but independently, and migration occurs among the population intermittently. A combination of breeder GA and parallel GA is known as the *distributed breeder genetic algorithm* (Mühlenbein and Schlierkamp-Voosen 1993). In a comparison between parallel GA and breeder GA, Mühlenbein (1993) states that "parallel GA models evolution which self-organises" but "breeder GA models rational controlled evolution".

Crossover

Many crossover operators have been developed in the GA literature. Here, four crossover operators (one-point, two-points, uniform, and even-odd) are reported from the literature. To disentangle the explication, assume that we have two individuals that we would like to crossover, $x = (x_1, x_2, x_3, \ldots, x_n)$ and $y = (y_1, y_2, y_3, \ldots, y_n)$ to produce two children, $c1$ and $c2$.

In *one-point crossover* (sometimes written 1-point) (Holland 1998), a cut point, p_1, is generated at random in the range $[1, n)$ and the corresponding parts to the right or left of the

cut-point are swapped. Assuming that $p_1 = 2$, the two children are formulated as $c1 = (x_1, x_2, y_3, \ldots, y_n)$ and $c2 = (y_1, y_2, x_3, \ldots, x_n)$. In *two-points crossover* (sometimes written 2-points) (Holland 1998; Jong 1975), two cut points, $p_1 < p_2$, are generated at random in the range $[1, n)$ and the two middle parts in the two chromosomes are interchanged. Assuming that $p_1 = 1$ and $p_2 = 5$, the two children are formulated as $cc1 = (x_1, y_2, y_3, y_4, y_5, x_6, \ldots, x_n)$ and $c2 = (y_1, x_2, x_3, x_4, x_5, y_6, \ldots, y_n)$. In *uniform crossover* (Ackley 1987), for each two corresponding genes in the parents' chromosomes, a coin is flipped to choose one of them (50-50 chance) to be placed in the same position in the child. In *even-odd crossover*, those genes in the even positions of the first chromosome and those in the odd positions of the second are placed in the first child and vice-versa for the second; that is, $c1 = (y_1, x_2, y_3, \ldots, x_n)$ and $c2 = (x_1, y_2, x_3, \ldots, y_n)$ assuming n is even.

Mutation

Mutation is a basic operator in GAs that introduces variation within the genetic materials, to maintain enough variations within the population, by changing the loci's value with a certain probability. If an allele is lost due to selection pressure, mutation increases the probability of retrieving this allele again. In our implementation, a repair operator is used to replace the conventional mutation operator to maintain the feasibility of the chromosomes.

6.5 Differential evolution

DE (Storn and Price 1995) is a branch of evolutionary algorithms developed by Rainer Storn and Kenneth Price in 1995 for optimisation problems with continuous decision variables. DE represents each variable's value in the chromosome with a real number. The approach works by creating a random initial population of potential solutions, where it is guaranteed that the value of each variable is within its boundary constraints. An individual is then selected systematically for replacement. Three different individuals are selected randomly as parents. One of these three individuals is selected as the main parent. Each variable in the main parent is changed with some probability while at least one variable should be changed. The change is undertaken by adding

let G denotes a generation, P a population of size M, and $x^l_{G=k}$ the l^{th} individual of dimension N in population P in generation k, and CR denotes the crossover probability

input $N, M \geq 4, F \in (0,1), CR \in [0,1]$, *and initial bounds:* $lower(x_i), upper(x_i), i = 1, \ldots N$

initialise $P_{G=0} = \{x^1_{G=0}, \ldots, x^M_{G=0}\}$ *as*

foreach *individual* $l \in P_{G=0}$

$x^l_{i,G=0} = lower(x_i) + random[0,1] \times (upper(x_i) - lower(x_i)), i = 1, \ldots, N$

evaluate every $x^l \in P_{G=0}$, $l = 1, \ldots, M$

$k = 1$

while *the stopping criterion is not satisfied* **do**

foreach $l \leq M$

randomly select $r_1, r_2, r_3 \in (1, \ldots, M), l \neq r_1 \neq r_2 \neq r_3$

randomly select $i_{rand} \in (1, \ldots, N)$

$$\forall i \leq N, x'_i = \begin{cases} x^{r_3}_{i,G=k-1} + F \times (x^{r_1}_{i,G=k-1} - x^{r_2}_{i,G=k-1}) & if \quad (random[0,1) < CR \wedge i = i_{rand}) \\ x^l_{i,G=k-1} & otherwise \end{cases}$$

$$x^l_{G=k} = \left\{ \begin{array}{l} x' \;\; if \;\; f(x') \leq f(x^j_{G=k-1}) \\ x^l_{G=k-1} \;\; otherwise \end{array} \right\}$$

$k = k + 1$

evaluate every $x^l \in P_{G=k}$, $l = 1, \ldots, M$

return $x = arg\max_l f(x^l), x^l \in P_{G=k}$, *the best encountered solution*

Figure 6.6: The differential evolution algorithm

to the variable's value in the main parent, a ratio of the difference between the two values of this variable in the other two parents. In essence, the main parent's vector is perturbed with the other two parents' vector. If the resultant vector is better than the one chosen for replacement, it replaces it; otherwise the chosen vector for replacement is retained in the population. Therefore, DE differs from GA in a number of points:

1. DE uses real number representation while GA uses binary, integer, or real number representation.

2. In GA, two parents are selected for crossover and the child is a recombination of its parents. In DE, three parents are selected for crossover and the child is a perturbation of one of these parents.

3. The new child in DE replaces a randomly selected vector from the population only if it is better than it. In canonical GA, children necessarily replace the parents.

The algorithm

To formally introduce DE, consider a multi-dimensional vector $x^l = (x_1, \ldots, x_N)^T$ representing a solution l. A population at generation $G = k$ is a vector of M solutions $(M > 4)$[2], $P_{G=k}$. The initial population, $P_{G=0} = \{x^1_{G=0}, \ldots, x^M_{G=0}\}$, is initialised as

$$x^l_{i,G=0} = lower(x_i) + rand_i[0,1] \times (upper(x_i) - lower(x_i)), l = 1, \ldots, M, i = 1, 2, \ldots, N \quad (6.8)$$

where M is the population size, N is the solution's dimension, and each variable i in a solution vector l in the initial generation $G = 0$, $x^l_{i,G=0}$, is initialised within its boundaries $(lower(x_i), upper(x_i))$. Selection is carried out to select four different solutions indexes $r_1, r_2, r_3, l \in [0, (M-1)]$. The values of each variable in the child are changed with some crossover probability, CR, to

$$\forall i \leq N, x'_i = \begin{cases} x^{r_3}_{i,G=k-1} + F \times (x^{r_1}_{i,G=k-1} - x^{r_2}_{i,G=k-1}) & if \quad (random[0,1) < CR \wedge i = i_{rand}) \\ x^l_{i,G=k-1} & otherwise \end{cases} \quad (6.9)$$

where $F \in (0, 1)$ is a problem parameter determining the amount the main parent is perturbed. The new solution replaces the old one if it is better than it and at least one of the variables should be changed (represented in the algorithm by randomly selecting a variable, $i_{rand} \in (1, N)$). After crossover, if one or more of the variables in the new solution are outside their boundaries, the following repair rule is applied

$$x^l_{i,G} = \begin{cases} \frac{x^l_{i,G} + lower(x_i)}{2} & if \quad x^l_{i,G} < lower(x_i) \\ lower(x_i) + \frac{x^l_{i,G} - upper(x_i)}{2} & if \quad x^l_{i,G} > upper(x_i) \\ x^l_{i,G} & otherwise \end{cases} \quad (6.10)$$

The DE algorithm is presented in Figure 6.6. Figure 6.7 depicts a graphical interpretation of the update rule for the differential evolution algorithm. It is clear from the figure that vector Xj is a perturbation of the parent X1 vector with some degree depending on the two parents X2 and X3.

6.6 Immune systems

In biological immune systems (Hajela and Yoo 1999), type-specific antibodies recognise and eliminate the antigens (*ie.* pathogens representing foreign cells and molecules). It has been

[2] M has to be greater than 4 since we select one vector for replacement and three different vectors as parents

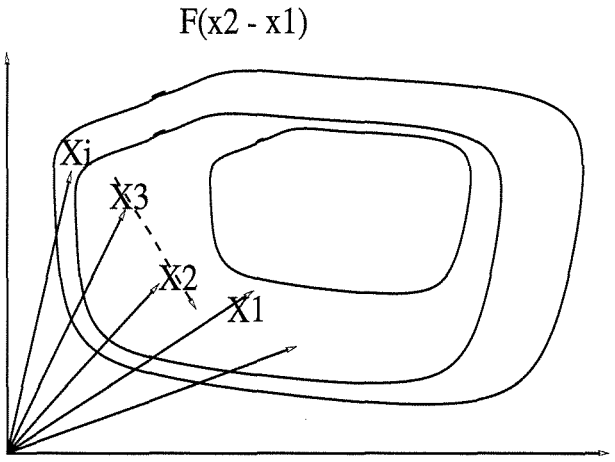

Figure 6.7: Differential evolution in the two dimensional space.

Two dimensional example of an objective function showing its contour and the process for generating Xj.

estimated that the immune system is able to recognise at least 10^{16} antigens; an overwhelming recognition task given that the genome contains about 10^5 genes. For all possible antigens that are likely to be encountered, the immune system must use segments of genes to construct the necessary antibodies. For example, there are between 10^7 and 10^8 different antibodies in a typical mammal. In biological systems, this recognition problem translates into a complex geometry matching process. The antibody molecule region contains a specialised portion, the paratope, which is constructed from amino acids and is used for identifying other molecules. The amino acids determine the paratope as well as the antigen molecules' shapes that can be attached to the paratope. Therefore, the antibody can have a geometry that is specific to a particular antigen.

To recognise the antigen segment, a subset of the gene segments' library is synthesised to encode the genetic information of an antibody. The gene segments act cooperatively to partition the antigen recognition task. In Immune, an individual's fitness is determined by its ability to recognise - through chemical binding and electrostatic charges - either a specific or a broader group of antigens.

The algorithm

An evolutionary approach is suggested by (Dasgupta 1998) for use in the cooperative matching task of gene segments. The approach (Dasgupta 1999) is based on genetic algorithms with a change in the mechanism for computing the fitness function. Therefore, in each GA generation, the top y% individuals in the population are chosen as antigens and compared against the population (antibodies) a number of times suggested (Dasgupta 1999) to be twice the population size. In each time, an antigen is selected at random from the set of antigens and compared to a population's subset. A similarity measure (assuming a binary representation, the measure is usually the hamming distance between the antigen and each individual in the selected subset) is calculated for all individuals in the selected subset. Then, the similarity value for the individual which has the highest similarity to the antigen is added to its fitness value and the process continues. The algorithm is presented in Figure 6.8. Different immune concepts inspired other computational models. For further information, the reader may wish to refer to (Dasgupta 1999).

6.7 Ant colony optimisation

ACO (Dorigo and Caro 1999) is a branch of a newly developed form of artificial intelligence called *swarm intelligence*. Swarm intelligence is a field which studies "the emergent collective intelligence of groups of simple agents" (Bonabeau et al. 1999). In insects which live in colonies, such as ants and bees, an individual can only do simple tasks on its own while the colony's cooperative work is the main reason behind the intelligent behaviour it shows.

Real ants are blind. However, each ant, while it is walking, deposits a chemical substance on the ground called *pheromone* (Dorigo and Caro 1999). Pheromone guides the future ants to make their way through and it evaporates with time. In a couple of experiments presented in (Dorigo et al. 1996), the complex behaviour of the ants' colony is illustrated. For example, Figure 6.9, a set of ants built a path to the food. An obstacle with two ends is then placed in their way where one end of the obstacle was more distant than the other. In the beginning, equal number of ants spread around the two ends of the obstacle. Since all ants have almost the same speed, the ants going through the nearest end of the obstacle return before the ants going by the farthest

let G denote a generation and P a population
initialise the initial population of solutions $P_{G=0} = \{x^1_{G=0}, \ldots, x^M_{G=0}\}$
evaluate every $x^l \in P_{G=0}$, $l = 1, \ldots, M$
compare_with_antigen_and_update_fitness$(P_{G=0})$
k=*1*
while *the stopping criteria is not satisfied* **do**
    select P' *(an intermediate population) from* $P_{G=k-1}$
    $P_{G=k} \leftarrow$ *crossover individuals in* P'
    mutate elements in $P_{G=k}$
    evaluate every $x^l \in P_{G=k}$, $l = 1, \ldots, M$
    compare_with_antigen_and_update_fitness$(P_{G=k})$
    $k = k + 1$
return $x = arg\max_l f(x^l), x^l \in P_{G=k}$, *the best encountered solution*

procedure *compare_with_antigen_and_update_fitness*$(P_{G=k})$
  antigen = top y% in $(P_{G=k})$
  $l = 0$
  while $l < 2 \times M$
    antibodies $\subset P_{G=k}$
    randomly select $y \in$ *antigen*
    find x *where similarity*$(y, x) = arg\max_{x'}$ *similarity*(y, x'), $x' \in$ *antibodies*
    add similarity(y, x) *to the fitness of* $x \in P_{G=k}$
    $l = l + 1$
end procedure

Figure 6.8: The immune system algorithm

end (differential path effect). With time, the amount of pheromone the ants deposit increases on the shortest path and more ants prefer this path. This positive effect is called *autocatalysis.* The difference between the two paths is called the *preferential path effect* and it is the cause of pheromone increase on each side of the obstacle since the ants following the shortest path will make more visits to the source than those following the longest path. Because of pheromone evaporation, pheromone on the longest path vanishes with time.

The algorithm

The *Ant System* (AS) (Dorigo et al. 1991) is the first algorithm based on the behaviour of real ants for solving combinatorial optimisation problems. The algorithm worked well on small problems but did not scale well for large scale problems (Bonabeau et al. 1999). Many algorithms

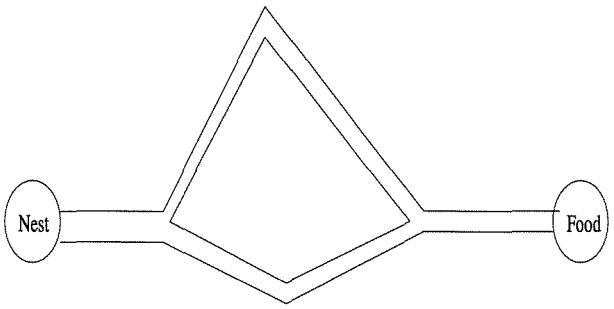

Figure 6.9: Autocatalysis and differential path length effects.

were developed to improve the performance of AS where two main changes were introduced. First, specialised local search techniques were added to improve the ants' performance. Second, ants deposit pheromone while they are building up the solution in addition to the normal rule of AS where an ant deposits pheromone after building up a solution. A generic version of the ACO algorithm is presented in Figure 6.10. In Figure 6.11, a conceptual diagram of the ACO algorithm is presented.

In the figures, the pheromone table is initialised with equal pheromones. The pheromone table represents that amount of pheromone deposited by the ants between two different states (*ie.* nodes in the graph). Therefore, the table is a square matrix with dimension depends on the number of states (nodes) in the problem. While the termination condition is not satisfied, an ant is created and initialised with an initial state. The ant starts constructing a path from the initial state to its pre-defined goal state (generation of solutions, Figure 6.11) using a probabilistic action choice rule based on the ant routing table (*ie.* a copy of the normalised pheromone matrix obtained by each ant). Depending on the pheromone update rule, the ant updates the ant routing table (re-inforcement). This takes place either after each ant constructs a solution (*online update rule*) or after all ants have finished constructing their solutions (*delayed update rule*). In the following two sub-sections, different methods for constructing the ant routing table and pheromone update are given.

Ant routing table (action choice rule)

The ant routing table is a normalisation of the pheromone table where the ant builds up its route by a probabilistic rule based on the pheromone available at each possible step and its

```
procedure ACO_heuristic()
    initialise pheromone_table
    while (termination_criterion_not_satisfied)
        foreach ant k do
            initialise_ant();
            M ← update_ant_memory();
            Ω ← a set of problem's constraints
            while (current_state ≠ target_state)
                A = read_local_ant-routing_table();
                P = compute_transition_probabilities(A,M,Ω);
                next_state = apply_ant_decision_policy(P, Ω);
                move_to_next_state(next_state);
                if (online_step_by_step_pheromone_update)
                then
                    deposit_pheromone_on_the_visited_arc();
                    update_ant_routing_table();
                M ← update_internal_state();
        if (online_delayed_pheromone_update)
        then foreach visited_arc do
            deposit_pheromone_on_the_visited_arc();
            update_ant_routing_table();
        die();
        Update_the_pheromone_table();
end procedure
```

Figure 6.10: Generic ant colony optimisation heuristic

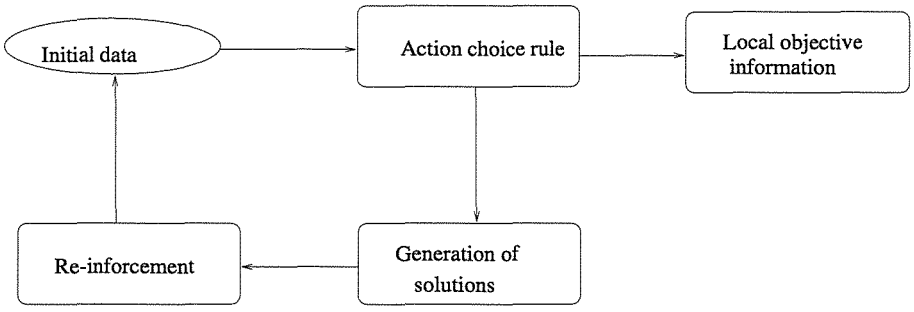

Figure 6.11: The ant algorithm.

memory. There are a number of suggestions in the literature for the probabilistic decision (a_{ij} is the element in row i column j in the matrix A (Figure 6.10) representing the probability that the ant will move from the current state i to the next potential state j). The first is the following rule:

$$a_{ij} = \frac{\tau_{ij}(t)}{\sum_{l \in N_i} \tau_{il}(t)} \tag{6.11}$$

Here, the ant utilises the pheromone information (τ_{ij} is the pheromone between the current state i and the next potential state j) only to decide on its next step (N_i is the set of possible transitions from state i). This rule does not require any parameter settings, however it is a biased exploratory strategy which can quickly lead to stagnation (Bonabeau et al. 1999). Another rule suggested by (Dorigo et al. 1991) is

$$a_{ij} = \frac{[\tau_{ij}(t)]^{\alpha}[\eta_{ij}]^{\beta}}{\sum_{l \in N_i}[\tau_{il}(t)]^{\alpha}[\eta_{il}]^{\beta}} \tag{6.12}$$

where we need two parameters α and β. The heuristic value η_{ij} is used for the intensification of search by means of a greedy behavior. For example, the heuristic value can be the immediate change in the objective resulting from increasing the value of a variable with 1 unit regardless of the effect of this increase on the overall solution. When $\beta = 1, \alpha = 0$, the algorithm behaves like local search and when $\beta = 0, \alpha = 1$ stagnation may occur as previously mentioned. A balance is usually required between α (the pheromone information's weight) and β (the local search's weight). However, this rule is computationally expensive because of the exponents. As an attempt to overcome this, (Dorigo and Gambardella 1997) suggested the following rule:

$$a_{ij} = \frac{[\tau_{ij}(t)][\eta_{ij}]^{\beta}}{\sum_{l \in N_i}[\tau_{il}(t)][\eta_{il}]^{\beta}} \tag{6.13}$$

where only one parameter β is used. However, the exponent is still an issue. More recently, the following rule is suggest for the quadratic assignment problem by (Maniezzo 1998):

$$a_{ij} = \frac{[\beta \times \tau_{ij}(t)][(1-\beta) \times \eta_{ij}]}{\sum_{l \in N_i}[\beta \times \tau_{il}(t)][(1-\beta) \times \eta_{il}]} \tag{6.14}$$

Here, only one parameter is required and the multiplication is computationally less expensive than the power.

Pheromone update (re-inforcement) rule

Each time a pheromone update is required, the ants use the following rule:

$$\tau_{ij}^{k}(t) \leftarrow (1-\rho)\tau_{ij}^{k}(t-1) + \Delta\tau_{ij}^{k}(t-1), \quad \forall i, j, k \tag{6.15}$$

where ρ is a discount factor for pheromone evaporation, ij represents a transition between state i and state j, and k is the number of ants. A number of suggestions were used in the literature

for calculating the rate of pheromone's change $\Delta\tau_{ij}^{k}(t-1)$. For example, in MMAS-QAP system,

$$\Delta\tau_{ij}^{k}(t-1) = \begin{cases} 1/J^{best} & \text{if ant } k \text{ moves from state } i \text{ to state } j \\ 0 & \text{otherwise} \end{cases} \tag{6.16}$$

where J^{best} is the objective value of the best solution found by the colony. We may note here that when the objective value increases, the rate of pheromone's change decreases, enabling search's intensification. Another suggestion to calculate $\Delta\tau^{k}(t-1)$ (Bonabeau et al. 1999) is

$$\Delta\tau_{ij}^{k}(t-1) = \begin{cases} \sum_{k\in K} C/J^{k} & \text{if ant } k \text{ moves from state } i \text{ to state } j \\ 0 & \text{otherwise} \end{cases} \tag{6.17}$$

where, K is the set of ants visited ij, J^{k} is the objective value of the solution generated by ant k, C is a constant representing a lower bound on the solutions that will be generated by the algorithm.

To summarise, at the beginning of the algorithm, the pheromone matrix is initialised. In each step, the pheromone matrix is normalised to construct the ant routing table. The ants generate a set of solutions (one solution per ant) by moving from a state to another using the action choice rule. Each element in the pheromone matrix is then updated using the pheromone update step and the algorithm continues.

6.8 Memetic algorithms

In his book, "The Selfish Gene", Richard Dawkins (1976) first coined the word *meme* to describe a unit of culture transmission as opposed to gene for genetic transmission. In the same timeframe, Lumsden and Wilson introduced a similar concept, *culturgen*, published later in their books "Genes, Mind, and Culture" (Lumsden and Wilson 1981) and "Promethean Fire" (Lumsden and Wilson 1983). The culturgen theory incorporates cultural transfer subject to epigenetic rules ("genetically determined procedures that direct the assembly of the mind, including the screening of stimuli by peripheral sensory filters, the internuncial cellular organising processes, and the deeper processes of directed cognition" (Lumsden and Wilson 1983)). Furthermore, they claimed that culture acts to slow the rate of genetic evolution, while both genetic and cultural evolution leads to major change in epigenetic rules over a minimum time of 1000 years. Examples

of memes are ideas, fashions, and any culture and behavioral unit that is learnt with a certain degree of fidelity. An example of an extremely powerful electronic meme is the computer-virus. Culture as defined by (Boyd and Richerson 1985) is:

> information capable of affecting individuals' phenotypes which they acquire from other conspecifics by teaching or imitation.

MAs are inspired by the previous idea and were first introduced in 1989 by Moscato (1989). In this work, it was suggested that cultural evolution can be a better working metaphor to escape from the biologically constrained thinking. The concept of cultural evolution in optimisation is a metaheuristic, where a heuristic is used to improve the solutions in an evolutionary algorithm following reproduction. MA has been applied extensively to many combinatorial optimisation problems (see (Moscato 1999) for a list). A generic version of MA is presented in Figure 6.12. In the figure, a local search procedure, $local\_search(x')$, is called after crossover and mutation. This procedure can be a hill-climbing or any other algorithm.

---

let G denotes a generation, P a population, and x^l the lth chromosome in P.
initialise the initial population of solutions $P_{G=0} = \{x^1_{G=0}, \ldots, x^M_{G=0}\}$
foreach $x^l \in P_{G=0}$ **do** $x^l \leftarrow local\_search(x^l)$
evaluate every $x^l \in P_{G=0}$, $l = 1, \ldots, M$
k=1;
while *the stopping criteria is not satisfied* **do**
    select P' (an intermediate population) from $P_{G=k-1}$
    $P_{G=k} \leftarrow$ *crossover elements in P'*
    foreach $x^l \in P_{G=k}$ **do** $x^l \leftarrow local\_search(x^l)$
    evaluate every $x^l \in P_{G=k}$, $l = 1, \ldots, M$
    mutate elements in $P_{G=k}$
    foreach $x^l \in P_{G=k}$ **do** $x^l \leftarrow local\_search(x^l)$
    evaluate every $x^l \in P_{G=k}$, $l = 1, \ldots, M$
    $k = k + 1$
return $x = arg\max_l f(x^l), x^l \in P_{G=k}$, *the best encountered solution*

Figure 6.12: A generic memetic algorithm

6.9 Constraints

Normally, optimisation problems contain constraints. In conventional optimisation theory, the problem may be solved in two stages. First, the algorithm searches for feasibility (satisfying the

constraint system). Second, while maintaining feasibility, the algorithm searches for optimality. Sometimes this is an easy task, if we have a single feasible region as in the case of linear programming. If the feasible region is discontinuous, this approach may not work. Constraints have received considerable attention in the literature of optimisation. Here, two main techniques for handling constraints are discussed: penalty function and repair methods. The choice of an appropriate technique is, sometimes, a problem-dependent task. For example, if the cardinality of the set of feasible solutions is small compared with the set of infeasible solutions, the penalty approach such as the death penalty may not be appropriate as demonstrated in the next section.

6.9.1 Penalty function

In this method, the basic goal is to define an objective function of two parts: the first is the original objective function (optimality criterion) and the second represents a measure of infeasibility (feasibility criterion). This means that the two components of the new objective function will compete together during the optimisation process. As such, this may be a problem since one component may subsume the other. Therefore, a weight factor for the measure of infeasibility is required to overcome this problem during the search. This weight factor, known as the *penalty* term/value, is the bottleneck of this technique. If the penalty value is under-estimated, feasibility may be broken and the algorithm converges to an infeasible solution. Over-estimating this term may cause problems to the heuristic technique (for example, in the case of GA, over-estimating the penalty term results in a GA-hard problem (Davis 1987; Riche et al. 1995)). The optimisation problem can be re-written as:

$$\text{Min. } f(x) + \gamma I(x).$$
$$\text{S.T.}$$
$$I(x) = \begin{cases} 0, if x \in \theta(x) \\ L, otherwise \end{cases} \tag{6.18}$$

where $\gamma > 0$ is a penalty term, and $I(x)$ is an evaluation function which returns 0 if x is a feasible solution and L, which is a measure of constraints violation, if x is infeasible. The amount of constraints violation may be measured in terms of the number of constraints violated, the amount of violation, or the amount of effort required to retrieve the feasibility (Dasgupta and

Michalewicz 1997).

Usually, the appropriate penalty value is learnt while the algorithm is searching for solutions (Richardson et al. 1989). A static penalty approach is suggested in Homaifar et al. (1994) where the user defines several levels of constraint violations, and associates with each level a suitable fixed penalty value, which increases when the level of violations increases. Annealing penalties (Michalewicz and Attia 1994) is an approach based on SA. In this method, the penalty value increases while the temperature decreases over time. Another penalty approach is adaptive penalties, introduced by Hadj-Alouane and Bean (1992), where it is determined while the search progresses. The penalty value decreases if all best individuals in the previous k generations were feasible and increases if they were infeasible; otherwise, the penalty value does not change. The importance of adaptive penalties is emphasised in Michalewicz (1996). Another interesting approach (Morales and Quezada 1998) is called the "death penalty" where an infeasible solution is evaluated in terms of the number of constraints it violates. The solution is not accepted if it exceeds a certain threshold on the number of violated constraints. Notice that this approach may prove inefficient when the cardinality of the set of feasible solutions is too small compared with that one of infeasible solutions (Michalewicz and Nazhiyath 1995).

In summary, when infeasibility is encountered, a penalty term can be added to the objective function to comprise a pressure on the search mechanism to retrieve feasibility again. Yet, the appropriate penalty value is a critical issue and none of the previous approaches is guaranteed to work all the time. Penalty functions are usually difficult to handle (Schoenauer and Xanthakis 1993) and they may not be the most suitable method for handling equality constraints (Coello 1999b).

6.9.2 Repair mechanisms

If repairing an infeasible solution is a cheap process, this approach can be a good one. In the literature of constraint satisfaction and local search algorithms (Lemaître and Verfaillie 1997; Minton et al. 1992), the use of a repair mechanism to retrieve broken feasibility is the conventional way to proceed. In the literature of GAs, it is shown that a repair operator results

in a better performance and is faster than other methods (Liepins and Vose 1990; Liepins and Potter 1991). GENOCOP III (Michalewicz and Nazhiyath 1995) is one of the most famous co-evolutionary systems which handle linear constraints using a repair operator. Repair operators can be found in many other studies such as Mühlenbein (1992), Michalewicz and Janikow (1991), Orvosh and Davis (1994), Riche and Haftka (1994), Riche et al. (1995), Xiao et al. (1997), and Xiao et al. (1996). Two main approaches are followed in this literature. The first is to use a repair algorithm in the solution's evaluation without replacing the infeasible solution with the repaired solution. Instead, the fitness of the repaired solution is used as the fitness of the infeasible solution. The idea here is that sometimes infeasible solutions may help to escape local optimum and may contains good bits. The second is to map the infeasible solution into a feasible solution and continuing the search from the new feasible solution. The problem with the second method is in the bias within the repair mechanism which may prejudice the search to a local optimum. This is not a problem in constraint satisfaction, since the objective is to reach a feasible solution without considering optimality. However, in optimisation this methodology may cause a premature convergence or being easily trapped in a local optimum, unless it is handled with randomisation as proposed in the following chapters.

6.10 Multi-objective optimisation

Normally, optimisation problems contain conflicting objectives. The literature of optimisation theory is rich in providing different methods for solving VOP. Unfortunately, these methods add a burden on the optimisation process, especially when problems are originally difficult to solve. There are three families of methods for solving VOP - ϵ-method, goal programming, and weighted-sum (aggregated) method.

The ϵ method (Ritzel et al. 1994) optimises the problem under each objective in order. After the optimisation of the first objective, the objective is added to the model as a constraint bounded with its optimal value $\pm$ a small value called ϵ. The second objective is then optimised under the original constraints and the new constraint obtained by adding the optimal solution of the first objective as a constraint. The process continues in a similar fashion. We need to alter the

values of ϵ to generate the set of pareto optimal solutions. The problem with this method is that it results in weak pareto-optimal solutions (Coello 1999a).

In its early stages, Archimedian goal programming approach (Charnes and Cooper 1961) was formulated within the framework of non-preemptive weights. In 1965, Ijiri (1965) introduced a preemptive approach. The Archimedian approach has been coined as *weighted goal programming* and the preemptive approach as *lexicographic goal programming.* A good introduction to goal programming can be found in (Ignizio 1976).

In the weighted-sum method (Kuhn and Tucker 1951), assume the vector of objective functions $F(x) = \{f_1(x), \ldots, f_k(x)\}$. If $W = \{w_1, \ldots, w_k\}$ is a normalised weight vector, the single-objective optimisation problem is formulated as

$$min \sum_{i=1}^{k} w_i \times f_i(x) \tag{6.19}$$

If one objective dominates another, the weights used in this optimisation process will not reflect the real importance of each objective. Therefore, scaling the objectives may be necessary (Coello 1999a).

$$min \sum_{i=1}^{k} w_i \times c_i \times f_i(x) \tag{6.20}$$

where c_i is a scaling factor, usually taken to be the reciprocal of the standard deviation of each objective over randomly generated sample.

6.11 Conclusion

In this chapter, the heuristic techniques, that will be used to solve the optimisation problem in the rest of the thesis, are presented. A wide range of techniques is covered, ranging from conventional techniques - such as simulated annealing, tabu search, and genetic algorithms - to more recent techniques such as ant colony optimisation and immune. In the next chapters, these techniques will be compared relative to their performance on the mate-selection problem. In addition, new techniques will be developed.

Chapter 7

Evolutionary Allocation Problem

Allocation is a common problem in *Operations Research* where the general idea is to allocate a limited number of finite resources to a limited number of objects. This problem can be solved using either general optimisation techniques such as *linear programming* or specialised techniques such as network optimisation. Usually the allocation is done for one time-slot but sometimes dynamic allocation is required. This chapter has two objectives:

1. Introducing and formulating a new type of dynamic allocation, *Evolutionary Allocation Problem* (EAP).

2. Estimating the problem complexity.

The chapter does not present a solution to the general problem although in the next chapters we will see how simplified versions of this problem can be solved. An introduction to allocation is presented in Section 7.1, followed by the problem importance in Section 7.2. In Section 7.3, the EAP's assumptions and advantages are stated, and the complexity of its search-space is discussed in Section 7.4 and conclusions are drawn in Section 7.5.

7.1 Introduction

The *allocation problem* is commonly found in daily activities. For example, in the beginning of each month we may need to allocate our salary to different expenses so that the monthly savings are maximum. The allocated values can be real or integer numbers. In the former, the problem is usually easier since techniques such as *linear programming* can handle it efficiently. The

problem becomes computationally expensive when the number of units allowed for allocation are constrained to be integer. In this case, techniques such as integer programming (Salkin and Mathur 1989) and constraint satisfaction (Gent and Walsh 1994; Hentenryck 1989) can solve problems of small to medium size.

When the dimension grows, specialised techniques can be more effective but limited in their scope. For example, if the problem is to assign a set of jobs to a set of machines so that every machine can process a single job, every job can be assigned to one machine only, and the total cost is to be minimised, then we deal with an *assignment problem* and a technique such as the *Hungarian algorithm* (Kuhn 1955) can efficiently solve it. Another type is the *transportation problem* where an integer number of units are required to be transported from a location to another so that the total cost is minimum. The transportation problem can be solved using an updated version of the Simplex method (Dantzig 1951). The underlying assumption of these techniques is that the problem is linear (linear objective with linear constraints). When the linearity assumption is relaxed, the problem becomes more difficult and more specialised techniques are required to solve it.

Papadimitriou et.al. (1982) show that the satisfiability problem and integer linear programming are NP-Complete problems. This is an interesting finding since it entails that until someone proves the unsolved dilemma NP=P, there cannot exist a polynomial algorithm which can efficiently solve these problems. This causes the research in these fields to be endless since none of the general algorithms can perform well on all problems, and specialised algorithms are required whenever a new problem arises.

In this chapter, a new type of allocation problem - the *Evolutionary Allocation Problem* - will be presented, which to my knowledge, has not yet been formulated in the operations research literature. The use of the term "evolutionary" in this context represents the evolving nature of the problem as opposed to an evolutionary algorithm for solving the problem. An evolutionary allocation problem can be defined formally as:

> Given a set of males, M, females, F, a number of years, Y, and criteria C, assuming the individuals are considered mature after G years from their date of birth, find the optimal set of mating-pairs between M and F for each year in Y in order to maximise

C. The progeny can be of either sex and they are available for allocation in subsequent years only when their age is greater than or equal to G.

The general representation will be illustrated with the assumption that the male individuals are bulls and the females are cows. Although this does not restrict the formulation, a fixed number of years is required for individuals from their date of birth to maturity. This is usually finite and to create a more understandable model, the domain of dairy industry is used as the model context. The mating of an animal can take place when it is one year old and the animal gives its first offspring at two years.

We do not know in advance whether a mating will result in a male or a female and this requires to be represented stochastically. Also, some of the animals may be culled and therefore cease to exist in later years. Additionally, the model must allow progeny to be unavailable for allocation until they become mature and therefore reproductive. Each animal is represented by a time-dependent binary vector component, which takes the value 1 only when the animal it represents is alive.

The problem is represented using a *stochastic multi-objective multi-stage decision model.* If the stochastic and the multi-objective components are ignored and selection of each individual in each generation is carried out independently and in advance, the problem is reduced to a dynamic transportation model. Here, it is assumed that the bull can be allocated to multiple dams. If the bull is allowed only to mate with at most one dam in a single generation, the problem is reduced to a dynamic assignment problem.

The difference between the conventional transportation model and the one presented here, is that source and destination nodes in the conventional model are known and are available for allocation in advance. In the current model, these nodes are non-deterministic. Non-determinism is handled in the model by attaching binary state variables to those nodes which determine the animal status (unborn, alive, reproductive, or dead) and reproductive behaviour in the generation.

7.2 Importance of the problem

The evolutionary allocation problem appears in many domains. The first is the economic domain which may be observed when a decision maker would like to model a dynamic economic system. In this case, investors and projects can be taken as the male and female individuals. Investors enter and leave the market, can invest in finite number of projects, and would like to compromise among conflicting objectives. Furthermore, the projects have a lifetime depending on whether they are long or short term investments and there is always a risk associated with the investment's outcome which represents the stochastic element here. A second domain is the financial domain. For example, in portfolio decisions, there may be a single source of money (maybe more) and many types of investments (shares, bonds, etc.). Additionally, every source of investment has two major characteristics, an interest and a risk which represent conflicting objectives. These problems can be seen as EAPs for one generation or can be extended to multi-generations.

The above examples are special cases of EAP. For instance, we may not need the parent-progeny relationship, therefore excluding the variables relating the progeny with the parents. Also, we may not need the concept of reproductive individuals since money does not need time to be usable. Nevertheless, if the outcome of an investment is insufficient to start a new project, this delayed investment may be considered equivalent to the concept of reproductive individuals.

Another domain is the dairy industry, the application domain of this thesis, where the farmer would like to allocate bulls to cows in order to optimise a number of objectives. Also, it can be applied to other animals such as lambs and pigs.

In summary, the EAP is an umbrella that can be customised to match many allocation problems in real life. The rest of this chapter is devoted to present a general formulation of this problem. This formulation can be customised to certain situations later on as demonstrated in chapter 9; there, it is customised to farmers using the artificial insemination program.

7.3 Model assumptions and advantages

The proposed model's assumptions are :-

1. Every animal has a unique index (position in state vectors) that it carries through all years whether or not it is yet to be born, alive, or dead.

2. Each mating results in a subsequent birth (the model does not allow for a probability of conception-failure). The offspring gender is determined stochastically.

The proposed model's advantages are :

1. It allows for overlapping generations; that is, the mother and the daughter can both be alive and giving birth in the same year.

2. It takes into account that animals are only reproductive after certain age.

3. There is no limit on the number of years to be optimised apart from the requirements of computer storage.

7.3.1 Nomenclature

Each year is equivalent to a stage in the model. The existence of reproductive animals, cows and bulls, is represented using the state variables DP and SP respectively. They also represent the availability of an animal, cow or bull, for mating. The existence of non-reproductive animals, one-year old cows and bulls, is represented using the state variables $D1$, and $S1$ respectively. The introduction of progeny into the herd is represented in relation to their parents and genders. These are four state variables, DD, SD, DS, and SS for the female child in relation to her mother and father and the male child in relation to his mother and father respectively.

The goal state is the optimal (best) herd composition over all years in the optimisation. Finally, the decision in each stage is the determination of whether an animal should be culled or mated. Furthermore, in the case of mating, which animal from the other sex should be involved in the mating. The variable M_{ij} represents these types of decisions between sire i and dam j. If the index of i is that of a special pseudo-sire $c(t)$, it means that the j^{th} dam is allocated for culling.

The same applies to the sire when $j = c(t)$ and the bull is paired with a special pseudo-dam.

In this model, a stage is taken to be 1 year. The years are denoted by $t = 1, 2, \ldots, T$, where T is the total number of years being modelled. We adopt the term "bull" generally for any male animals in the herd not yet mated. We reserve the term "sire" specifically for male animals that have been mated. Thus $S1$ defines young bulls and SP defines reproductive bulls some of which may actually be sires already. The vector $X(t)$ identifies those bulls that have been mated in year t and so they may more appropriately be called sires. Similar remarks apply to the vector $Y(t)$ which identifies for cows (corresponding to bulls) and dams (corresponding to sires).

If the model is to be solved using *simulation* techniques, at the start of simulation time unit t, all bulls and cows that are reproductive are reflected by the vectors SP and DP. Thus, if bull i is mature (that is, was conceived in the beginning of time $t-2$, was born at the end of the same year, and so is older than one unit of simulation time, may or may not have offspring but has not been culled) then $SP_i(t) = 1$. If at time t, it is selected for mating then the i^{th} component of X, $X_i(t)$ is set to 1, otherwise $X_i(t)$ is set to 0. At simulation time $t+1$, $SP_i(t+1)$ is set to 1 if $S1_i(t) = 1$ (that is, the bull has just become reproductive at $t+1$ and will be now available for mating) and in addition $X_i(t) = 1$ (that is, the bull was reproductive at time t and was not selected for culling). Accordingly, the variable $X_i(t)$ is a transition variable used to hold components for the purpose of helping update the new set of reproductive bulls $SP(t+1)$. In a strict mathematical sense the vector X is superfluous, however it is very convenient for purposes of structuring the set of transitions in the model. Similar reasons apply to the corresponding transition vector Y, used for cows. Figure 7.1 depicts the scope of each state variable when a conception takes place.

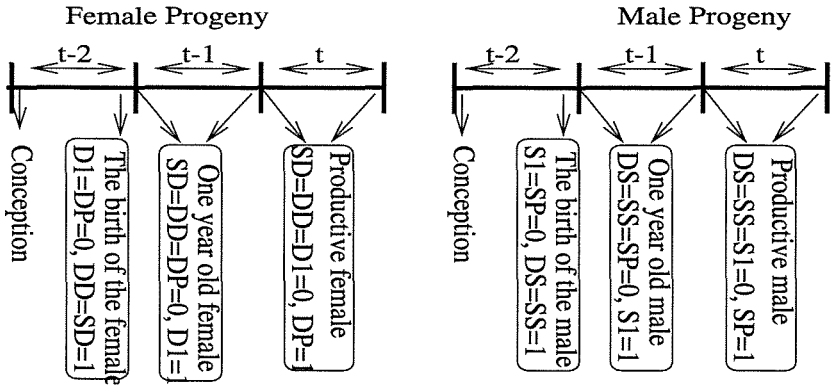

Figure 7.1: The state variables' scope in the model before time t.

The list of user defined parameters:-

T:	Total number of years.
NT:	Number of traits.
S:	Total number of bulls summed over all generations.
D:	Total number of cows summed over all generations.
$S_{max}(t)$:	The maximum number of matings per sire at time t.
$D_{max}(t)$:	The maximum number of matings per dam at time t.
$S_{cull}(t)$:	Number of sires to be culled at time t.
$D_{cull}(t)$:	Number of dams to be culled at time t.
$N_{mate}(t)$:	The number of matings required at time t.
$c(t)$:	Dummy variable to be allocated to any culled animal that is, an animal that is not selected for mating, and therefore is to be culled, is assigned a pseudo-mating to $c(t)$.
λ_{sinbr}:	The cost of 1 unit inbreeding.
λ_{linbr}:	The cost of 1 unit coancestry divided by twice the number of matings.
b_k:	The price of one unit of trait k.
a_k:	The economic value of trait k.
$\mathbf{1}$:	A column vector of ones.
A:	Matrix with additive genetic numerator relationships over all generations.
G_{ki}:	The expected additive genetic merit of trait k for animal i.

P_{ki}: The phenotypic value of trait k for animal i.

The list of state variables:-

$S1_i(t)$: Bull i at time t is one year old (and non-reproductive).

$SP_i(t)$: Bull i at time t is reproductive ($age > 1$).

$D1_j(t)$: Cow j at time t is one year old (and non-reproductive).

$DP_j(t)$: Cow j at time t is reproductive ($age > 1$).

$DD_{ij}(t+1)$: The density function of a Bernoulli distribution where

$$DD_{ij}(t+1) = f(x) = \begin{cases} 1, & if\, the\, stochastic\, variable\, x \geq 0.5 \\ 0, & otherwise \end{cases}.$$

If $DD_{ij}(t+1)$ is 1 then at $t+1$ dam i become the mother of cow j, resulting from a mating at t. x is a uniformly distributed independent random variable.

$DS_{ij}(t+1)$: The density function of a Bernoulli distribution where

$$DS_{ij}(t+1) = f(x) = \begin{cases} 1, & if\, the\, stochastic\, variable\, x \geq 0.5 \\ 0, & otherwise \end{cases}.$$

If $DS_{ij}(t+1)$ is 1 then at $t+1$ dam i become the mother of bull j, resulting from a mating at t. x is a uniformly distributed independent random variable.

$SD_{ij}(t+1)$: The density function of a Bernoulli distribution where

$$SD_{ij}(t+1) = f(x) = \begin{cases} 1, & if\, the\, stochastic\, variable\, x \geq 0.5 \\ 0, & otherwise \end{cases}.$$

If $SD_{ij}(t+1)$ is 1 then at $t+1$ sire i become the father of cow, resulting from a mating at t. x is a uniformly distributed independent random variable.

$SS_{ij}(t+1)$: The density function of a Bernoulli distribution where

$$SS_{ij}(t+1) = f(x) = \begin{cases} 1, & if\, the\, stochastic\, variable\, x \geq 0.5 \\ 0, & otherwise \end{cases}.$$

If $SS_{ij}(t+1)$ is 1 then at $t+1$ sire i become the father of bull j, resulting from a mating at t. x is a uniformly distributed independent random variable.

The list of decision variables are:

$X_i(t)$: A binary variable set to 1 if bull (reproductive male) i is alive in time t and is not culled; otherwise 0.

$Y_j(t)$: A binary variable set to 1 if cow (reproductive female) j is alive in time t and is not culled; otherwise 0.

$M_{ij}(t)$: A binary variable set to 1 if the i^{th} sire is mated with the j^{th} dam in time t; otherwise 0. M_{ij} is an element in the mating matrix M.
An extra row and column is added to represent culling.

7.3.2 The objective function

In this section, some interesting objectives are introduced from the dairy industry view point. These objectives can be changed independently of the constraint systems. It is guaranteed that the constraint systems are valid regardless of the objective's nature by isolating the domain specific components in the objective function, omitting the general constraints in an evolutionary allocation problem. Therefore, there is not domain specific knowledge in the system of constraints. It may be added here that each sub-objective can be transformed into a constraint by setting the appropriate bound(s) on it.

A typical sub-objective to be maximised in a breeding program is the genetic gain. Kinghorn (1987) finds that mate-selection has no value when the genetic traits are additive. In this case, mating the selected individuals randomly will result in the optimal solution (at least for the next stage); that is, mate randomly the best bulls with the highest genetic values with the best cows. If there is an interaction between parents, the objective function becomes nonlinear, *eg.* due to dominance, heterosis, inbreeding depression, or other nonlinear breeding phenomena. In addition, for the longer term, the objective function is nonlinear due to the effect of co-ancestry.

In designing the breeding sub-objectives, a compromise between short and long term objectives

is required. Short term objectives will apply to those criteria which will contribute to the short term (the following year or two). For example, culling cows with low phenotypic production value will increase the average production per cow within the farm. Two short term objectives are considered: the profit of not culling an animal in the current period taken to be its expected production profit in the following stage, and the short term inbreeding depression represented with the average inbreeding (in producing animals) multiplied by the cost of 1 unit inbreeding depression.

Two long term objectives are defined: genetic gain and long term inbreeding (coancestry). Long term gain also is affected by genetic variation. Matings can create more or less variation and therefore affect future merit. The impact of improving the genetic makeup in a herd appears after a number of years (*eg.* in dairy cattle, after one generation, which is about 5 years). Long term inbreeding, known as coancestry (Wray and Goddard 1994), is the second long term objective. The idea here is simply to minimise the level of relationship between the animals within each year so that inbreeding is minimised on the long run.

The four sub-objectives for short and long term planning can be formulated as follows:

1. $O1$: the first short term objective representing the production index:

$$Maximise \quad O1 = \sum_{t=1}^{T} \sum_{j=1}^{D} (\sum_{k=1}^{NT} b_k \times P_{kj}(t)) \times Y_j(t). \tag{7.1}$$

   In this sub-objective a production index, $\sum_{k=1}^{NT} b_k \times P_{kj}(t)$, is calculated by multiplying the price of trait k, b_k, by the phenotypic value of this trait for animal j, $P_{kj}(t)$, at time t, where NT is the number of traits. The index's value is significant only if the animal is alive and reproductive; that is, $Y_j(t) = 1$. We may note that the value of production is meaningful only for the female and consequently, the males are not included in this objective.

2. $O2$: the second short term objective representing short term inbreeding:

$$Minimise \quad O2 = \sum_{t=1}^{T} \lambda_{sinb} \times ([X^t(t), Y^t(t)]^t \times \ (Diag(A) - \mathbf{1})). \tag{7.2}$$

In this sub-objective, $Diag(A)$ returns the diagonal elements of the numerator relationship matrix as a column vector and by subtracting from it a vector of ones, $\mathbf{1}$, the result is simply the inbreeding coefficient for each animal which, if multiplied by the vector $[X^t(t), Y^t(t)]^t$, the result will be the total inbreeding in generation t. Multiplying this value by the cost of one-unit inbreeding, λ_{sinb}, results in the total short-term inbreeding cost/penalty. The matrix A can be constructed easily using the algorithm of Henderson (1975b) where the matrices DS, SD, DD, and SS provide the pedigree information required for constructing A.

3. $O3$: the first long term objective representing the breeding values:

$$Maximise \quad O3 = \sum_{t=1}^{T}\sum_{i=1}^{S} X_i(t) \times \sum_{k=1}^{NT}(a_k \times G_{ki}(t)) + \sum_{t=1}^{T}\sum_{j=1}^{D} Y_j(t) \times \sum_{k=1}^{NT}(a_k \times G_{k(S+j)}(t)). \tag{7.3}$$

In this sub-objective, a selection index, $\sum_{k=1}^{NT}(a_k \times G_{ki}(t))$, is calculated by multiplying the economic value of trait k, a_k, by the expected genotypic value of this trait for animal i, $G_{ki}(t)$, at time t. The index value is significant only for alive animals (males and females), $X_i(t) = 1$ and $Y_j(t) = 1$.

4. $O4$: the second long term objective representing long term inbreeding:

$$Minimise \quad O4 = \sum_{t=1}^{T} \lambda_{linb} \times [\sum_{j=1, j\neq c(t)}^{D} M_{ij}(t), \ (\sum_{i=1, i\neq c(t)}^{S} M_{ij}(t))^t] \times \mathbf{A} \times$$
$$[(\sum_{j=1, j\neq c(t)}^{D} M_{ij}(t))^t, \ \sum_{i=1, i\neq c(t)}^{S} M_{ij}(t)]. \tag{7.4}$$

In this sub-objective, the coancestry relationship is calculated by multiplying a row vector of the proportional contribution of each animal, $[\sum_{j=1,j\neq c(t)}^{D} M_{ij}(t), \ (\sum_{i=1,i\neq c(t)}^{S} M_{ij}(t))^t]$, times the numerator relationship matrix, times the transpose of the vector representing the

contribution of each animal. If this value is multiplied by the cost/penalty of coancestry divided by twice the number of matings, λ_{linb}, the resultant value is the cost of long term inbreeding (der Werf 1990). The two components in the square brackets represent a concatenation of two vectors. Each component is derived from matrix M by summing either the rows (*ie.* $i = 1 \ldots S$) or the columns (*ie.* $j = 1 \ldots D$), which yields a column or row vector respectively.

The problem can also be formulated as a single objective stochastic multi-stage decision model by introducing a set of preferential weights, α, β, γ, and δ,. The negative weights are assigned to transform a minimisation sub-objective to a maximisation one. In this case, the objective function will be,

$$Maximise \ \alpha \times O1 + \beta \times O2 + \gamma \times O3 + \delta \times O4, \quad \alpha, \gamma \geq 0, \beta, \delta \leq 0 \tag{7.5}$$

7.3.3 Constraints

There are two types of constraints in the model: explicit and implicit or logical constraints. Explicit constraints are marked (*Explicit*). The model involves a considerable number of logical constraints to be satisfied by the state variables. These constraints fall into categories, we call A, B, ..., F, with the constraints within a category being somewhat similar. A special category (*logical*) is designated for logical constraints not associated with the state variables. If we consider state variables in their vector or matrix form (for example, $X = (X_1, X_2, ...)$), then each constraint affects a number of state variables that tend to occur in pairs. As an aid to visualise the constraints, we have presented in Figure 7.2 a graph with nodes labelled with the state variables and arcs labelled with constraint categories. The arcs connecting pairs of variables (nodes) are labelled with the relevant constraint category. For example, the arc labelled "A1" joining nodes M (the mating matrix) and DD (the mother-daughter relationship matrix) refers to a constraint category between M and DD that is similar to constraints between M and DS, SS and SD which are also labelled "A1", "A2", and "A2" in the figure. The arrows in the figure are used to suggest causation. For example, the matrix DD follows as a result of a mating via the matrix M producing female offspring. Therefore, the arc is directed from M to DD.

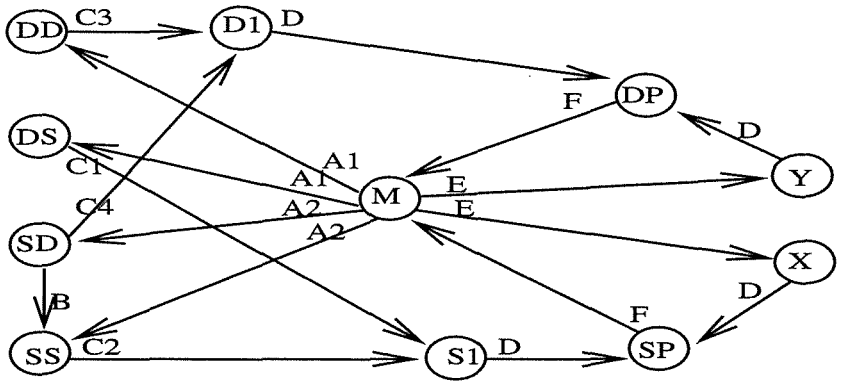

Figure 7.2: The logical relationships between the model's variables

1. The number of matings for each sire (dam) is not allowed to exceed the maximum number of matings allowed for a sire (dam) in year t (the matings take place between vectors $SP(t)$ (productive sires) and $DP(t)$ (productive dams) as illustrated before. (Category *Explicit*)

$$\sum_{i=1,i\neq c(t)}^{S} M_{ij}(t) \leq D_{max}(t), \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.6}$$

$$\sum_{j=1,j\neq c(t)}^{D} M_{ij}(t) \leq S_{max}(t), \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.7}$$

2. The total number of allocations should equal the total number of matings required. (Category *Explicit*)

$$\sum_{i=1,i\neq c(t)}^{S} \sum_{j=1,j\neq c(t)}^{D} M_{ij}(t) = N_{mat}(t), \quad t = 1 \ldots T. \tag{7.8}$$

3. The total number of bulls/cows allocated for culling should equal the total number of culling required. All cows, which are non-mated in a generation, are culled at the end of that generation. (Category *Explicit*)

$$\sum_{j=1,j\neq c(t)}^{D} M_{c(t),j}(t) = D_{cull}(t), \quad t = 1 \ldots T. \tag{7.9}$$

$$\sum_{i=1,i\neq c(t)}^{S} M_{i,c(t)}(t) = S_{cull}(t), \quad t = 1 \ldots T. \tag{7.10}$$

4. A sire or dam that is allocated for mating cannot be allocated for culling in the same years. (Category *logical*)

$$M_{i,c(t)}(t) \times \sum_{j=1,j\neq c(t)}^{D} M_{ij}(t) = 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.11}$$

$$M_{c(t),j}(t) \times \sum_{i=1,i\neq c(t)}^{S} M_{ij}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.12}$$

5. A logical constraint preventing the mating between the two special culling nodes in each year. This constraint is essential to prevent cycling. (Category *logical*)

$$M_{c(t),c(t)}(t) = 0, \quad t = 1 \ldots T. \tag{7.13}$$

6. Each sire (dam) mated at the beginning of year t has a number of progeny in the end of the year equal to the number of its matings. (Category A1 and A2)

$$\sum_{i=1,i\neq c(t)}^{S} M_{ij}(t) - \sum_{k=1}^{D} DD_{jk}(t) - \sum_{l=1}^{S} DS_{jl}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.14}$$

$$\sum_{j=1,j\neq c(t)}^{D} M_{ij}(t) - \sum_{k=1}^{D} SD_{ik}(t) - \sum_{l=1}^{S} SS_{il}(t) = 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.15}$$

7. If a mating M_{ij} occurred, the offspring gender in the year for both the sire and the dam is the same.

$$M_{ij}(t) - \sum_{k=1}^{D} DD_{jk}(t) \times SD_{ik}(t) - \sum_{l=1}^{S} DS_{jl}(t) \times SS_{il}(t) = 0$$

$$, \quad i = 1 \ldots S, j = 1 \ldots D, t = 1 \ldots T. \tag{7.16}$$

8. For all sires in each year, the number of male progeny equals the number of female progeny. Here it is required that the actual number of males and females offspring equal the expected number. However, to count for the case where the total number of progeny is an odd number, it is required that the difference between the number of males and females progeny to be less than or equal to one. (Category B)

$$\sum_{i=1}^{S}\sum_{k=1}^{D} SD_{ik}(t) - \sum_{i=1}^{S}\sum_{l=1}^{S} SS_{il}(t) \leq 1, \quad t = 1 \ldots T. \tag{7.17}$$

9. Progeny conceived in the current year (t) will be one-year-old non-reproductive individuals in the next year (t+1) and each child has precisely one mother and one father. (Category C)

- Each male child has one mother.

$$\sum_{l=1}^{D} DS_{li}(t) = S1_i(t+1), \quad i = 1 \ldots S, t = 1 \ldots (T-1). \tag{7.18}$$

- A one-year-old male child in year t cannot be a new child of any dam in year t.

$$S1_i(t) + \sum_{l=1}^{D} DS_{li}(t) \leq 1, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.19}$$

- A reproductive male child in year t cannot be a new child of any dam in year t.

$$SP_i(t) + \sum_{l=1}^{D} DS_{li}(t) \leq 1, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.20}$$

- Each male child has one father.

$$\sum_{l=1}^{S} SS_{li}(t) = S1_i(t+1), \quad i = 1 \ldots S, t = 1 \ldots (T-1). \tag{7.21}$$

- A one-year-old male child in year t cannot be a new child of any sire in year t.

$$S1_i(t) + \sum_{l=1}^{S} SS_{li}(t) \leq 1, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.22}$$

- Each female child has one mother.

$$\sum_{l=1}^{D} DD_{lj}(t) = D1_j(t+1), \quad j = 1 \ldots D, t = 1 \ldots (T-1). \tag{7.23}$$

- A one-year-old female child in year t cannot be a new child of any dam in year t.

$$D1_j(t) + \sum_{l=1}^{D} DD_{lj}(t) \leq 1, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.24}$$

- A reproductive female child in year t cannot be a new child of any dam in year t.

$$DP_j(t) + \sum_{l=1}^{D} DD_{lj}(t) \leq 1, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.25}$$

- Each female child has one father.

$$\sum_{l=1}^{S} SD_{lj}(t) = D1_j(t+1), \quad j = 1 \ldots D, t = 1 \ldots (T-1). \tag{7.26}$$

- A one-year-old female child in year t cannot be a new child of any sire in year t.

$$D1_j(t) + \sum_{l=1}^{S} SD_{lj}(t) \leq 1, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.27}$$

10. Any reproductive bull/cow in the next year is either a one year old bull/cow in the current year, or it is a sire/dam in the current year and *has not been culled.* This also forces a bull/cow to be either reproductive or not. (Category D)

$$SP_i(t+1) = S1_i(t) + X_i(t), \quad i = 1 \ldots S, t = 1 \ldots (T-1). \tag{7.28}$$

$$SP_i(t) + S1_i(t) \leq 1, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.29}$$

$$DP_j(t+1) = D1_j(t) + Y_j(t), \quad j = 1 \ldots D, t = 1 \ldots (T-1). \tag{7.30}$$

$$DP_j(t) + D1_j(t) \leq 1, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.31}$$

11. A flag constrains $X_i(t)$ to refer to sires that are not culled in year t. If sire i had a real mating in year t then we must force $X_i(t)$ to be 1. Similar results apply to $Y_j(t)$ for dams. (Category F)

$$(1 - X_i(t)) \times \sum_{j=1, j \neq c(t)}^{D} M_{ij}(t) = 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.32}$$

$$-X_i(t) + \sum_{j=1, j \neq c(t)}^{D} M_{ij}(t) \geq 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.33}$$

$$(1 - Y_j(t)) \times \sum_{i=1, i \neq c(t)}^{S} M_{ij}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.34}$$

$$-Y_j(t) + \sum_{i=1, i \neq c(t)}^{S} M_{ij}(t) \geq 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.35}$$

12. The bulls/cows are available for allocation in year t if and only if they are reproductive in year t. In the first constraint, if bull i is mated or culled, it must be reproductive and $SP_i(t)$ forced to 1. In the second constraint, if bull i is not mated or culled then it is non-reproductive and $SP_i(t)$ is forced to 0. The same interpretation applies for the subsequent two constraints for a cow. (Category H)

- If bull i is allocated then it must be reproductive.

$$(1 - SP_i(t)) \times \sum_{j=1}^{D} M_{ij}(t) = 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.36}$$

- If it is reproductive, then it must be allocated (even for culling).

$$-SP_i(t) + \sum_{j=1}^{D} M_{ij}(t) \geq 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.37}$$

- If cow i is allocated then it must be reproductive.

$$(1 - DP_j(t)) \times \sum_{i=1}^{S} M_{ij}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.38}$$

- If it is reproductive, then it must be allocated (even for culling).

$$-DP_j(t) + \sum_{i=1}^{S} M_{ij}(t) \geq 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.39}$$

- The progeny born in year t must be guaranteed not to exist as individuals in previous years (*ie.* 0 ... $(t-1)$).

$$\sum_{k=1}^{D} DS_{ki}(t) \times \sum_{l=1}^{(t-1)} X_i(l) = 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.40}$$

$$\sum_{k=1}^{S} SS_{ki}(t) \times \sum_{l=1}^{(t-1)} X_i(l) = 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{7.41}$$

$$\sum_{k=1}^{D} DD_{kj}(t) \times \sum_{l=1}^{(t-1)} Y_j(l) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.42}$$

$$\sum_{k=1}^{S} SD_{kj}(t) \times \sum_{l=1}^{(t-1)} Y_j(l) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{7.43}$$

7.4 Model complexity

This model can be solved either as a Stochastic Multi-objective Multi-stage decision Model or expanded and solved as a stochastic multi-objective binary nonlinear model.

In the former, the number of variables in each year is $D^2 + S^2 + 2D \times S + 3D + 3S + D \times S$, which simplifies to $(D+S)^2 + 3 \times (D+S) + D \times S$. These values are derived from Equations 7.6 to 7.43. There are up to $16D + 16S + D \times S + 5$ constraints. The search space in each year will be approximately $2^{(D+S)^2+3\times(D+S)+D\times S}$. For example, if we have 200 dams and 10 sires and we wish to optimise for 5 years, there will be 46,730 variables in each year with at most 5,365 constraints, and approximately search space size of 10^{14067}.

In the latter, the number of variables is $T \times ((D+S)^2 + 3 \times (D+S) + D \times S)$ with $16 \times T \times (D+S) + T \times D \times S + 5 \times T - 3 \times (S+D)$ constraints. The search space will be $2^{T\times((D+S)^2+3\times(D+S)+D\times S)}$. In the previous example, there will be 233,650 variables in all years with 26,195 constraints, and

approximately search space size of 10^{70335}.

7.5 Conclusion

This chapter emphasises the formulation aspect of the third thesis sub-objective; formulating and solving the version of the mate-selection problem to be solved in this thesis, where a stochastic multi-objective multi-stage decision model was formulated for our generic mate-selection problem. The model with its very high complexity, is definitely not solvable by conventional optimisation techniques. The complexity presented here assumes our formulation, and raises a number of questions.

Q: Is the proposed formulation, the best one?

A: One may argue that there are better formulations. For example, why do we not have a single vector for all dams, where each cell in the vector is an index (*eg.* -1 for culling, 0 for birth, 1 for one year old, and 2 for reproductive)? The same may apply for the bulls. This is an interesting way to combine the binary vectors $D1$, DP, and Y into a single vector and accordingly may reduce the search space. Let us call the proposed vector of multiple values V. The question now is how to formulate the constraint that if $V(t)$ is 1 then $V(t+1)$ should be 2? The answer is simple; introduce a flag (binary variable) to indicate that the value of $V(t)$ is 1 and use this flag to force the value of $V(t+1)$ to be 2 (notice that the constraint $2 \times V(t) - V(t+1) = 0$ is not a valid choice here because when $V(t) = 0$, $V(t+1)$ should be 0 as well but the animal can live many years after being mature). But we have introduced a binary variable for this logical equation and we require different ones for each logical equation. Essentially, this means that we paid much more than what we saved!

It is not claimed here that this is the best formulation that can ever be found. Formulation is an art. Nevertheless, many different ways to formulate the problem have been investigated and this was the best method found.

Q: Do we need a complex formulation? We build simulation models and all logical constraints are controlled by simple "if...then..." rules. Why do we require this complicated model if the problem can be programmed in few lines? Do we need to waste over 20 pages to present the problem?

A: The quote in the beginning of this chapter by Albert Einstein answered these questions already. Life is simple but controlling it is not. The fact that this problem can be coded into a computer program or can be simulated does not contradict our finding that the search space is enormous. The first useful contribution of the proposed formulation is that no one can claim a tractable algorithm for solving the problem and reaching an optimal solution. The second is to understand the dimension of the problem we are dealing with instead of dreaming with optimality. This may save a lot of time and wasted efforts. The third is that it provides a formal representation as a rational starting point to solve a complex problem. The fourth contribution is that it embraces the complete picture, where one can start with a simplified version and then increase the complexity gradually once a suitable algorithm is found.

In the following chapters, customised versions of this model are presented for farmers depending completely on artificial insemination bulls. It will also be shown that the reduction of this model to single stage is a quadratic transportation problem (quadratic objective with linear constraint). The single stage model will be solved using genetic algorithms in Chapter 8 as well as the customised version of the multi-stage model in Chapter 9.

Chapter 8

Genetic Algorithm Applied to the Single-stage Model

This chapter aims at formulating a single stage mate-selection model and then finding the best set of GA operators that result in a prompt effective solution for the problem. This set of GA operators is essential for the next chapter in the process of solving the multi-stage model. In Section 8.1, the formulation of the evolutionary allocation problem, presented in Chapter 7, will be customised for farms dependent on the artificial insemination program; where natural mating is not allowed. In Section 8.2, a genetic algorithm design for the single-stage model is presented followed by a number of experiments with the aim of identifying a set of genetic algorithm operators that reach the best solution found quickly and reliably in Section 8.3.

8.1 A single stage model

In Chapter 7, the evolutionary allocation problem formulation was shown. It was found that the problem is very complex, both in reality (for an animal breeder) and in its mathematical representation. In this chapter, the problem is simplified to a degree by assuming female offspring and sires are coming from an artificial insemination service with all sires genetically unrelated to the initial set of cows. Also, a stage is taken to be two years to reduce the complexity of the model by eliminating those transitions and state variables which keep track of the animal age.

In this section, the multi-stage model will be reduced to a single-stage model that will be solved

and used as a basis for solving the former. In the single-stage model, a considerable number of variables and constraints will be removed. All transition variables and all state variables except the matrix M are obliterated from the model. The single-stage model is then[1]:

$$Maximise\ \ \alpha \times O1 + \beta \times O2 + \gamma \times O3 + \delta \times O4, \quad \alpha, \gamma \geq 0, \beta, \delta \leq 0 \tag{8.1}$$

where

$$O1 = \sum_{j=1}^{D} \sum_{k=1}^{NT} b_k \times P_{kj} \times \sum_{i=1, i \neq c}^{S} M_{ij} \tag{8.2}$$

$$O2 = \lambda_{sinb} \times E^t \times \ (Diag(A) - \mathbf{1}) \tag{8.3}$$

$$O3 = \sum_{j=1}^{D} \sum_{i=1, i \neq c}^{S} M_{ij} \times \sum_{k=1}^{NT} (a_k \times G_{k(S+j)}) \tag{8.4}$$

$$O4 = \lambda_{linb} \times [\ \sum_{j=1, j \neq c}^{D} M_{ij},\ \ (\ \sum_{i=1, i \neq c}^{S} M_{ij})^t] \times \mathbf{A} \times [(\ \sum_{j=1, j \neq c}^{D} M_{ij})^t,\ \ \sum_{i=1, i \neq c}^{S} M_{ij}] \tag{8.5}$$

subject to:

$$\sum_{i=1}^{S} M_{ij} \leq 1, \quad j = 1 \ldots D \tag{8.6}$$

$$\sum_{j=1}^{D} M_{ij} \leq S_{max}, \quad i = 1 \ldots S \tag{8.7}$$

$$\sum_{i=1, i \neq c}^{S} \sum_{j=1}^{D} M_{ij} = N_{mat} \tag{8.8}$$

$$\sum_{j=1}^{D} M_{cj} = D_{cull} \tag{8.9}$$

$$M_{ij} \in \{0, 1\}, \quad i = 1 \ldots S, j = 1 \ldots D \tag{8.10}$$

Several changes have been introduced to the model. Since no culling is allowed for sires, the vector E is introduced in the second objective with dimension $S + D + number\ \ of\ \ progeny$. The first $S + D$ elements in E are 0_s and the others are 1_s. Therefore, the short term inbreeding is, as usual, a function of the progeny. The term concerning the genotypic values for sires is excluded from the third objective since again, the farmer's own sires are not considered here.

[1]Because the model is reduced to a single-stage one, only explicit constraints remain.

The single-stage model is now reduced to a quadratic transportation model (*ie.* quadratic objective function with linear constraints). The source of the quadratic term is $O4$, the coancestry term. Actually, this model is highly non-linear if we consider how the matrix A is generated. Recalling from Chapter 2, A is generated by a set of recursive functions over the family tree of the animals. In the rest of this chapter, this model will be solved using GA. Assuming 200 dams and 10 sires, the search space is 10^{660}.

8.2 Genetic algorithm for the single-stage model

To present the application of GA for solving the single-stage model, a number of issues still need to be addressed. These are representation, crossover operators, and the repair operator (*ie.* method of maintaining the constraint-system's feasibility). The repair operator is effectively replacing the mutation operator, since it introduces variations to the model when the chromosome's feasibility is broken.

8.2.1 Representation

The selected representation for the problem will be introduced followed by a discussion of some alternatives and the extent of their pertinence. In the chosen representation, the dams and sires are randomly assigned a unique index between $0-(D-1)$ and $0-(S-1)$ respectively. The chromosome is represented with an array of dimension equal to the number of dams. Each position j in the array is analogous to dam j in the model and each cell in the array can take one of $S+2$ integer values, where S is the number of sires and the additional two values are -1 for culling and -2 for not selected. For example, having the value 3 in cell 1 signifies that the dam number 1 is allocated to sire number 3. This representation guarantees the feasibility of Constraint 8.6 since there is only one cell per dam. Consequently, every dam will be bound to a single decision (mating, culling, or no-action). In contrast, Constraints 8.7, 8.8, and 8.9, may be broken. Therefore, a strategy to retrieve the feasibility will be explained in Section 8.2.3. Assuming 200 dams and 10 sires, the search space, using the proposed representation, is reduced from 10^{660} to 10^{208}. A typical chromosome in the GA for the single stage model is as shown in Figure 8.1.

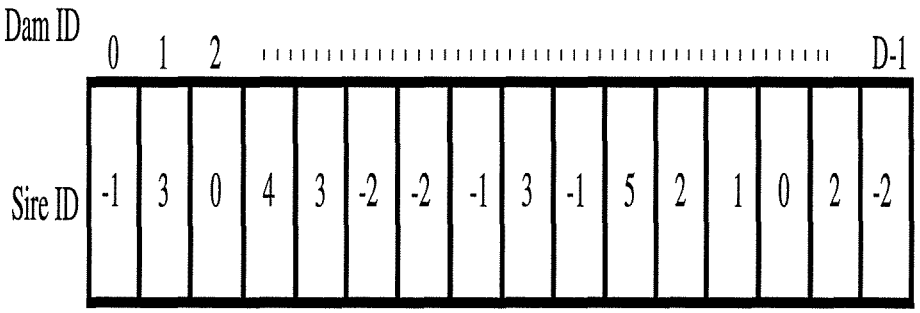

Figure 8.1: The data structure for the chromosome in the single-stage model.

This representation is similar to Hayes et al. (1997) except that Hayes et al. coded all animals that were not mated as 0; therefore representing redundancy in the representation.

One among many other possible ideas for an effective representation, in terms of memory, is to have a two-dimensional chromosome. The array's columns represent dams, the rows represent sires, and each cell ij takes either 1 - if the dam i is mated to sire j - or 0 - if no allocation is made. Culling a dam is represented by a dummy sire/row. Although, this is a natural way to represent the mating matrix M in the model, it will exhaust the memory. Sparse representation or bit manipulation may save some memory here although it is still expensive compared to the selected representation.

Another way is to have a two-dimensional chromosome where the columns represent sires and the rows represent the maximum number of mating per sire. Culling is represented by a dummy sire with the number of cows assigned to it equal to the total number of culling required. Again this requires more memory than the selected representation. For example, presume that there are 1000 dams and 100 sires: the maximum number of mating per sire is 20, the total number of mating required is 500, and the number of culling required is 500. In this representation, a two-dimensional array of size 100×20 plus a one-dimensional array for culling of size 500 are required; that is, 2500 integer locations are occupied in the memory. In the selected representation, the chromosome will occupy only 1000 integer locations in the memory, which is 60% less.

8.2.2 Crossover

Additional to the crossover operators mentioned in Chapter 6, a biased version of the uniform crossover is proposed, *gene-based crossover*. In gene-based crossover, the goal here is to calculate the contribution of each gene to the total fitness, and to then use the relative gene fitness as a crossover probability. The reason is that we assume in gene-based crossover an additive model; where the overall fitness of a chromosome is the summation of the individual fitness of each gene. It is essential to distinguish between fitness distribution as introduced here, and the *fitness distribution analysis* (Fogel and Ghozeil 1996) recently presented in the literature. Fitness distribution analysis is used to predict the variation operators' effect in the population, mainly for continuous optimisation. Here, fitness distribution means distributing the total chromosome fitness among its genes. This does not necessarily require that the components of the fitness function be separable as will be exemplified soon. The algorithm for the gene-based crossover is given in Figure 8.2.

```
re-distribute the two chromosomes' fitness on all genes
if the first chromosome's fitness > the second
   begin
      foreach gene, g1, in the first chromosome and its corresponding gene in the second chromosome, g2
         if fitness(g1) > fitness(g2)
         then choose g1 or g2 with a probability proportion to their fitness
         else assign 50% chance for g1 and g2 to be chosen
   end
else
begin
   foreach gene, g1, in the first chromosome and its corresponding gene in the second chromosome, g2
      if fitness(g1) < fitness(g2)
      then choose g1 or g2 with a probability proportion to their fitness
      else assign 50% chance for g1 and g2 to be chosen
end

function fitness(gi)
   sum = 0
   add to sum the genotypic, phenotypic, and inbreeding values of the animal
   add to sum the animal's contribution in the coancestry term
   return sum
end function
```

Figure 8.2: The gene-based crossover operator.

The distribution of the chromosome's fitness among its genes is easy if the objective function

is a linear combination of the genes (*ie.* the function is separable). For example, assume that the objective function of a chromosome is $\sum sin(x_i)$, where x_i is the value of gene i. This is a nonlinear objective but it is separable in terms of the genes and therefore easily distributed among the genes. By contrast, if the objective is not a linear combination of the genes, separability becomes quite difficult. Every gene in the single-stage model represents an allocation of a dam to a decision; that is, selection for mating or culling, or not selected. The only non-separable component in the objective function is the coancestry term (Equation 8.5), all the remaining components of the objective functions are linear. The coancestry term is quadratic and can be distributed in the following way. Assume the following quadratic function in four variables x_1, x_2, x_3, and x_4:

$$\begin{pmatrix} x_1 & x_2 & x_3 & x_4 \end{pmatrix} \begin{pmatrix} 1.2 & 0.1 & 0.1 & 0.1 \\ 0.1 & 1.2 & 0.1 & 0.1 \\ 0.1 & 0.1 & 1.2 & 0.1 \\ 0.1 & 0.1 & 0.1 & 1.2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

If the first term on the left is multiplied by the matrix that is similar to the numerator relationship matrix, the result is:

$$\begin{pmatrix} 1.2x_1 + 0.1x_2 + 0.1x_3 + 0.1x_4 \\ 0.1x_1 + 1.2x_2 + 0.1x_3 + 0.1x_4 \\ 0.1x_1 + 0.1x_2 + 1.2x_3 + 0.1x_4 \\ 0.1x_1 + 0.1x_2 + 0.1x_3 + 1.2x_4 \end{pmatrix}^t \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

The total value of this multiplication is a function of x_1 to x_4. The first term reflects the contribution of x_1 as a function of the relationship between x_1 and the other variables, $1.2x_1 + 0.1x_2 + 0.1x_3 + 0.1x_4$. In the coancestry term, this is equivalent to the relationship between the first selected animal and all those selected for mating. This term is used as the contribution of x_1 in the objective. In a similar manner, the other three terms are chosen for x_2 to x_4 in order.

8.2.3 Repair operator: constraint satisfaction algorithm

In the GA implementation for solving the single-stage model, a repair operator is used to maintain the solution's or chromosome's feasibility. Feasibility may be broken after crossovering two feasible solutions or at the start of each run when the population is randomly initialised. The

repair operator is unbiased in the sense that all changes are made by random selection, which has a similar effect to mutation. The algorithm is presented in Figure 8.3.

```
count the number of allocations, alloc_i, per each sire, i, and the total number of culling, Cull
foreach sire i
   if alloc_i > maximum_number_of_sire_allocations then
      while alloc_i ≠ maximum_number_of_sire_allocations do
         randomly select one of the dams allocated to i
         assign the value −2 to it
         alloc_i = alloc_i − 1
next i
if Cull > number_of_allowed_culling then
   while Cull ≠ number_of_allowed_culling do
      randomly select a dam j
      if j has a value −1 then assign −2 to j, Cull = Cull − 1
else if Cull < number_of_allowed_culling then
      while Cull ≠ number_of_allowed_culling do
         randomly select a dam j
         if j has a value −2 then assign −1 to j
         else if j has a value > −1 then
               alloc_i = alloc_i − 1, i is the sire allocated to j
               assign −1 to j
               Cull = Cull + 1
count the total number of mating, Mat
if Mat > number_of_allowed_mating then
   while Mat ≠ number_of_allowed_mating do
      randomly select a dam j
      if j has a value > −1 then
         alloc_i = alloc_i − 1, i is the sire allocated to j
         assign −2 to j
         Mat = Mat − 1
if Mat < number_of_allowed_mating then
   while Mat ≠ number_of_allowed_mating do
      randomly select a dam j
      if j has a value −2 then
         randomly select a sire i, alloci < maximum_number_of_sire_allocations
         assign i to j
         Mat = Mat + 1
         alloc_i = alloc_i + 1
```

Figure 8.3: The repair operator.

The algorithm starts with counting the number of allocations for each sire. A loop is then constructed, over all sires. If a sire exceeds the maximum number of allowed mating per sire, the excess is eliminated by randomly selecting a dam from those mated to this sire and assigning to

it the symbol -2, denoting a *no action* decision. This process is repeated until all sires meet the maximum allowed mating per sire constraint. The next step is to calculate the total number of dams selected for culling. If this number exceeds the number of culling requested by the user, a dam which is assigned to culling is selected at random and the symbol -2 is then assigned to it. The step is repeated until the total number of dams assigned for culling equals the number of culling required. If the total number of culling is less than that determined by the user, a dam is selected at random. If the value assigned to this dam is -2, it is set to -1 and the total number of culling is increased by one. If the value assigned to this dam is greater than -1 - the dam is selected for mating and is being assigned to a bull - the number of mating for the bull allocated to this dam is reduced by one, the total number of mating is reduced by one, and the dam is assigned -1. The process is repeated until the total number of culling equals the number of culling required by the user. Then, the total number of mating in the chromosome is calculated. If the total number of mating is greater than the number of mating required by the user, a dam which is being assigned to a bull is selected at random and assigned -2. The total number of mating is then reduced by 1 and the algorithm loops until the total number of mating equals the number of mating required by the user.

If the total number of mating is less than the number of mating required by the user, a dam which is assigned -2 is selected at random and a bull that has not reached maximum number of mating per bull, is chosen at random and is assigned to this dam. The total number of mating is increased by one and the algorithm loops until the total number of mating is equal to the number of mating required by the user.

8.3 Experiments

8.3.1 The data simulation model

Ten artificial herds were generated at random with different seeds and evolved for 20 years. The following steps were repeated for each of the ten herds. In year 0, 40 sires and 60 dams were randomly generated then mated for 20 years. In each year, 20 dams were selected at random for culling and 27 were selected at random for mating to simulate a random mating strategy, with

a pedigree structure between them built up. In the end of the 20 years, each herd contained 640 animals (40 sires and 600 cows) with 200 dams still alive (*ie.* available for mating).

The ten initial herds were simulated for a realistic Australian Holstein Friesian breed. The following equation (see Equation 2.17) was used in year 0 to randomly sample the phenotype Y_{ijk} (note that this is not the same variable $Y_j(t)$ presented in the multi-stage mathematical model) for S sires and D dams:-

$$Y_{ijk} = \mu + YS_i + A_j + PE_j + E_{jk} \tag{8.11}$$

where, μ is the herd mean, YS_i is the season-year fixed effects where $i = 1, \ldots, 5$, A_j is the additive genetic effect for animal j, PE_j is the permanent environmental effect for animal j, and E_{jk} is the residual effect for the k^{th} record for animal j. Here, each animal has a single record.

The heritability (h^2) and repeatability (r) were 0.25 and 0.40 respectively. The herd mean (μ) was 5000. The five year-season effects were -100, 0, 100, 200, 300. The phenotypic (σ_P), additive (σ_A), permanent environmental (σ_{PE}), and residual (σ_E) standard deviations were calculated using the following equations:

$$\sigma_P = 0.1 \times \mu = 500 \tag{8.12}$$

$$\sigma_A = \sqrt{(h^2)} \times \sigma_P \tag{8.13}$$

$$\sigma_{PE} = \sqrt{(r - h^2)} \times \sigma_P \tag{8.14}$$

$$\sigma_E = \sqrt{(1 - r)} \times \sigma_P \tag{8.15}$$

The matrix $\sigma^2(BV, EBV)$ is a symmetric matrix with the main diagonal's elements $(1,1) = (2,2) = \sigma_a^2$ and the elements $(2,1),(1,2) = r^2 \times \sigma_a^2$. The EBVs for the sires and dams were sampled by taking a Cholesky decomposition (Mrode 1996) of this matrix and multiplying the resultant triangular matrix with a vector of two random variables (each of them sampled independently from a Gaussian distribution ($N(0,1)$).

Each dam was allocated a year-season effect at random, where the pseudo-random number was sampled from $U(0,1)$. The permanent environmental and residual effects were sampled from

$N(0, \sigma^2_{PE})$ and $N(0, \sigma^2_E)$ respectively.

Each dam selected for mating was assigned a bull at random. The BVs for the progeny, assumed to be heifer, were calculated using the following equation,

$$Progeny \quad BV \quad = 0.5 \times (Sire \quad BV + Dam \quad BV) + \phi \tag{8.16}$$

where the Mendelian sampling, ϕ, is $N(0, \sigma^2(\phi))$. $\sigma^2(\phi) = 0.5 * \sigma^2_A * (1 - 0.5(F_s + F_d))$, where F_s and F_d are the parents' inbreeding coefficients. This is equation was used to simulate real animals representing the candidates available for mating.

8.3.2 Experimental design and objective

The main objective of this experiment is to select a set of GA operators that are capable of reaching a good solution quickly and reliably. The speed is measured in terms of the number of GA-generations, for a fixed population size, required to reach the best solution within a run of fixed length, 1000 GA-generations. We may note that the time is a critical factor here since the farmer is not willing to wait weeks until the results come out of the computer. The reliability is measured in terms of the stability of these operators among a number of runs with different weight initialisations and among a set of randomly generated problems. The average of the average performances of the ten runs is calculated for both measures.

In the experiments, a canonical GA (progeny always replace their parents) is used as the reproduction strategy. Three selection operators (roulette wheel with linear scaling, Stochastic Baker, and modified tournament - see Chapter 6) are tested each with five different crossover operators (1-point, 2-points, uniform, even-odd, and gene-based) to comprise 15 combinations. The GA is run using each of these combinations on the ten herds, each of which is run ten times with different seeds; that is, 1500 runs, each run is 1000 GA-generations long. The repair operator is used in all runs. An elitism strategy (*ie.* the best solution in one GA-generation is cloned to the next) is adopted. The maximum number of mating allowed per sire are 5, the number of required culling 50, and the total number of required mating 100. The weights for each objective were 0.01 for the phenotypic objective, 1 for the genotypic objective, -200 for the inbreeding

objective, and -1 for the coancestry objective. These weights were selected after 20 initial runs to overcome the problem of magnitude for each objective. Therefore, the the four objectives have actually the same value while the differences between the weights reflect the magnitude of each objective. A different strategy to overcome this problem will be discussed in the following chapter.

8.3.3 Results and discussion

Two criteria are used to evaluate the results: the number of GA-generations elapsed to find the best solution within 1000 GA-generations, and the average best solution value. The first criterion measures the speed, and the second quantifies the operators' ability to reach a good solution in a fixed number of GA-generations. The average of the number of GA-generations to find the best solution, and the average values of the best solution found at GA-generation 1000 for the population over the averages of ten runs with different seeds $\pm$ the standard deviation are shown in Table 8.1.

As can be seen from Table 8.1 in the third column and row 1 through 10, gene-based crossover outperforms all crossover operators when using fitness proportionate and Stochastic Baker selection operators. Notwithstanding, 1-point and 2-points crossover are better with the modified tournament selection. Also, it was noticed that the gene-based crossover operator is always outperforming the uniform crossover operator, which indicates that the bias introduced by the gene-based crossover improved the conventional uniform crossover operator in this problem. Nevertheless, it is outperformed by the 1-point and 2-points crossover when the modified tournament selection operator is used. However, it can be seen from Figures 8.4 8.5, that the gene-based crossover performs better in the first 100 GA-generations but the 1-point operator also then improves. In the same figures, the convergence to the best solution over 1000 GA-generations in the ten runs is shown for gene-based crossover, using fitness proportionate and Stochastic Baker selection operators, and 1-point crossover using modified tournament selection. The variations among the ten runs (in terms of the standard deviations of the best solution found in each run) were small; therefore suggesting that there is a consistency in the behaviour among different runs. This is very important since it indicates that the behaviour of the three combinations of operators is not sensitive to the initial seed. Also, the previous trends were consistent for the

other nine herds. Therefore, one can conclude that the operators' performance for this problem is stable.

In summary, the choice is between the 1-point and 2-points crossover with modified tournament selection. This choice is because, on the average, there is little difference between the best solution found by both operators as can be seen from Table 8.1 - rows 12 and 13 respectively. Since there is not much difference in the computations required for both of them, it was decided to adopt the 1-point crossover with modified tournament selection operator, for subsequent GA experiments in subsequent chapters, since it has the highest average (over the ten herds, 20810 $\pm$ 2440 compared to 20760 $\pm$ 2500 for two-points crossover operator). Furthermore, the standard deviation is lower than that for the 2-point crossover. It is clear that we did not need to try more than 2 points crossover since the solution did not improve with the increase in the number of crossover points.

Table 8.1: The average results of ten GA runs for one of the ten herds

Selection	**Crossover**	**Iterations to Best**	**Fitness of the Best**
Fitness proportion	1-point	940 $\pm$ 34	17915 $\pm$ 689
	2-points	945 $\pm$ 45	18714 $\pm$ 588
	uniform	770 $\pm$ 201	15112 $\pm$ 439
	even-odd	215 $\pm$ 176	14625 $\pm$ 2165
	gene-based	852 $\pm$ 133	19423 $\pm$ 266
Stochastic Baker	1-point	965 $\pm$ 38	20889 $\pm$ 431
	2-points	908 $\pm$ 175	20971 $\pm$ 437
	uniform	928 $\pm$ 53	20721 $\pm$ 458
	even-odd	225 $\pm$ 111	15593 $\pm$ 2122
	gene-based	963 $\pm$ 25	22306 $\pm$ 247
Modified Tournament	1-point	913 $\pm$ 76	23152 $\pm$ 205
	2-points	921 $\pm$ 44	23235 $\pm$ 200
	uniform	892 $\pm$ 102	21554 $\pm$ 225
	even-odd	68 $\pm$ 23	15701 $\pm$ 1941
	gene-based	864 $\pm$ 166	20852 $\pm$ 324

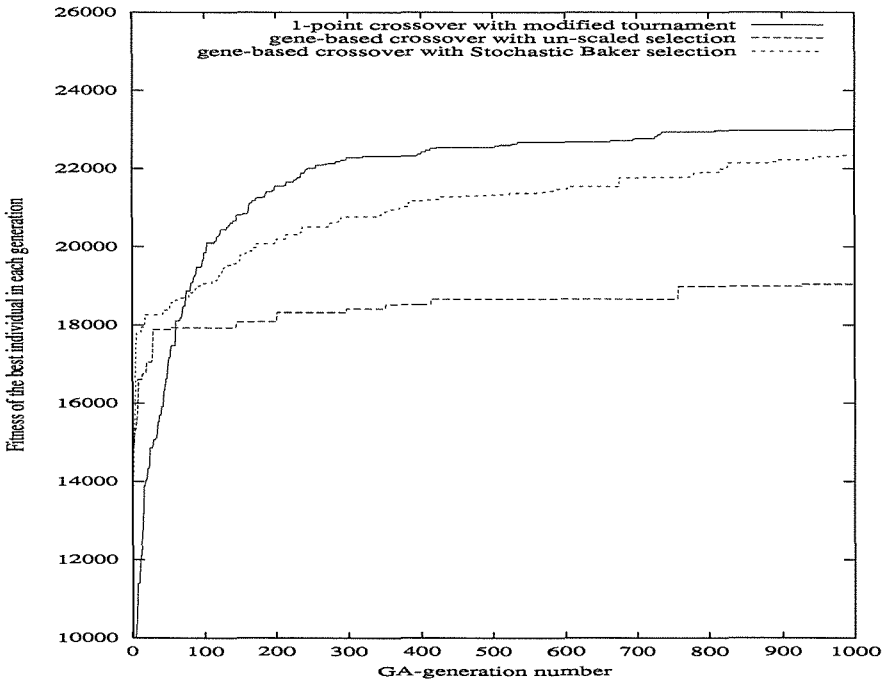

Figure 8.4: The trajectories of the best solution over 1000 GA-generations for a single run.

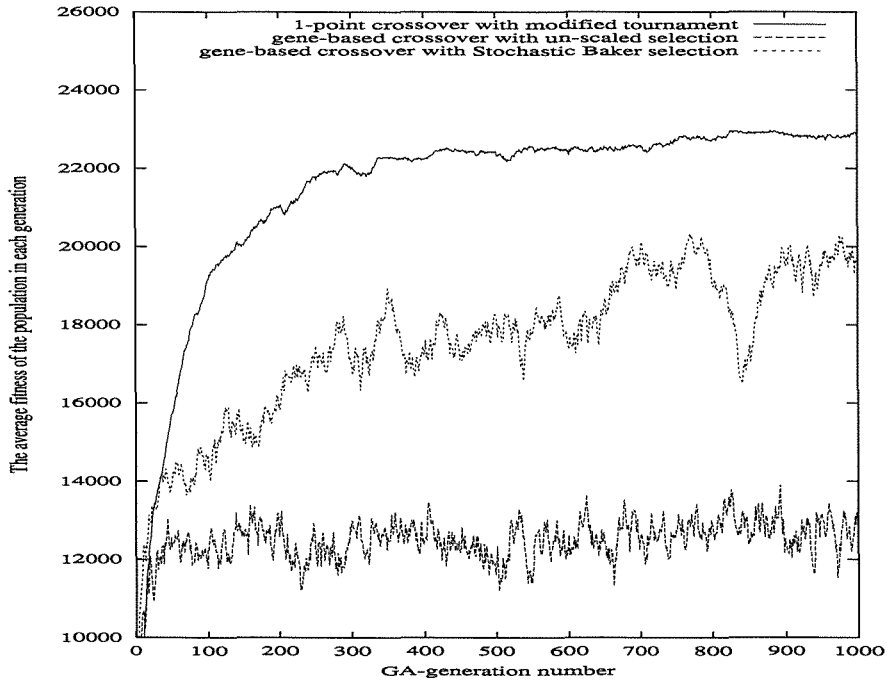

Figure 8.5: The trajectories of the average population fitness over 1000 GA-generations for a single run.

8.4 Conclusion

This chapter emphasises the solution of the single-stage mate-selection problem - that is being discussed in the previous chapter - as a step to solve the multi-stage mate-selection problem

which is the third thesis sub-objective; formulating and solving the mate-selection problem. The single-stage mate-selection problem is solved using genetic algorithms. The problem's solution is represented using a one-dimensional array and a repair operator is developed to maintain the feasibility of each solution-array. Three selection operators and five crossover operators are compared. The proposed gene-based crossover operator performes the best with fitness proportion and Stochastic Baker selection operators while the one-point crossover operator performes the best overall. It is also found that the performance of all operators is stable over all problems and initialisations.

Chapter 9

Solving the Multi-stage Mate-selection Problem

In this chapter, the formulation of the evolutionary allocation problem, presented in Chapter 7, will be customised for farms only using the artificial insemination program, where natural mating is not allowed. The problem is solved for five stages and it will be shown that the complexity is reduced although still high. In Section 9.1, the customisation of the EAP model to farms using the artificial insemination program is shown. The experimental design is introduced in Section 9.2. Different strategies for solving the model are then presented in Sections 9.4 to 9.5, 9.6, 9.7, 9.8, 9.9, 9.10, 9.11, and 9.12. Section 9.13 presents a summary of the best result found in each experiment and an overall comparison between the proposed solution strategies.

9.1 Customisation of the multi-stage model

In the previous chapter, the assumptions of the multi-stage model were set. In summary, the farmer uses only artificial insemination bulls, a stage is two years, and all the progeny are assumed to be females. It is worth mentioning here that a stage is taken to be two years to reduce the complexity of the model by eliminating those transitions and state variables which keep track on the animal age. The multi-stage model is solved for five stages but the farmer is given the results of the first stage only. This can be seen as a mate-selection index which discounts the future impact of current allocations (see next chapter). The reason for that is, giving the farmer a mate-selection schedule for the next five stages (*ie.* ten years) is associated with high

risk such as the gender of progeny, death of animals, and failure of conception. The advantages of the general model are still valid for the customised multi-stage model presented in this chapter.

Equations 7.10 to 7.13 are not required any more since males are artificial insemination bulls. Equations 7.17 to 7.22, 7.28 to 7.29, 7.32 to 7.33, 7.36 to 7.37, and 7.40 to 7.41 are excluded since male progeny are not allowed. The customised multi-stage model for farms using the artificial insemination program is similar to the one presented in Chapter 7 with the previous modifications. For clarity, the complete model follows. However, the relations in this model have been previously presented in Chapter 7.

$$Maximise\ \ \alpha \times O1 + \beta \times O2 + \gamma \times O3 + \delta \times O4, \quad \alpha, \gamma \geq 0, \beta, \delta \leq 0 \tag{9.1}$$

where

$$Maximise \quad O1 = \sum_{t=1}^{T} \sum_{j=1}^{D} (\sum_{k=1}^{NT} b_k \times P_{kj}(t)) \times Y_j(t). \tag{9.2}$$

$$Minimise \quad O2 = \sum_{t=1}^{T} \lambda_{sinb} \times ([X^t(t), Y^t(t)]^t \times \ (Diag(A) - \mathbf{1})). \tag{9.3}$$

$$Maximise \quad O3 = \sum_{t=1}^{T} \sum_{j=1}^{D} Y_j(t) \times \sum_{k=1}^{NT} (a_k \times G_{k(S+j)}(t)). \tag{9.4}$$

$$Minimise \quad O4 = \sum_{t=1}^{T} \lambda_{linb} \times [\sum_{j=1}^{D} M_{ij}(t), \ (\sum_{i=1, i\neq c(t)}^{S} M_{ij}(t))^t] \times \mathbf{A} \times [(\sum_{j=1}^{D} M_{ij}(t))^t, \sum_{i=1, i\neq c(t)}^{S} M_{ij}(t)]. \tag{9.5}$$

subject to:

$$\sum_{i=1, i\neq c(t)}^{S} M_{ij}(t) \leq 1, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.6}$$

$$\sum_{j=1}^{D} M_{ij}(t) \leq S_{max}(t), \quad i = 1 \ldots S, t = 1 \ldots T. \tag{9.7}$$

$$\sum_{i=1, i\neq c(t)}^{S} \sum_{j=1}^{D} M_{ij}(t) = N_{mat}(t), \quad t = 1 \ldots T. \tag{9.8}$$

$$\sum_{j=1}^{D} M_{c(t),j}(t) = D_{cull}(t), \quad t = 1 \ldots T. \tag{9.9}$$

$$M_{c(t),j}(t) \times \sum_{i=1, i \neq c(t)}^{S} M_{ij}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.10}$$

$$\sum_{i=1, i \neq c(t)}^{S} M_{ij}(t) - \sum_{k=1}^{D} DD_{jk}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.11}$$

$$\sum_{j=1}^{D} M_{ij}(t) - \sum_{k=1}^{D} SD_{ik}(t) = 0, \quad i = 1 \ldots S, t = 1 \ldots T. \tag{9.12}$$

$$M_{ij}(t) - \sum_{k=1}^{D} DD_{jk}(t) \times SD_{ik}(t) = 0, \quad i = 1 \ldots S, j = 1 \ldots D, t = 1 \ldots T. \tag{9.13}$$

$$DP_j(t) + \sum_{l=1}^{D} DD_{lj}(t) \leq 1, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.14}$$

$$DP_j(t) + \sum_{l=1}^{S} SD_{lj}(t) \leq 1, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.15}$$

$$DP_j(t+1) = \sum_{k=1}^{D} \sum_{l=1}^{S} DD_{kj}(t) SD_{kj}(t) + Y_j(t), \quad j = 1 \ldots D, t = 1 \ldots (T-1). \tag{9.16}$$

$$(1 - Y_j(t)) \times \sum_{i=1, i \neq c(t)}^{S} M_{ij}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.17}$$

$$-Y_j(t) + \sum_{i=1, i \neq c(t)}^{S} M_{ij}(t) \geq 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.18}$$

$$(1 - DP_j(t)) \times \sum_{i=1}^{S} M_{ij}(t) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.19}$$

$$-DP_j(t) + \sum_{i=1}^{S} M_{ij}(t) \geq 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.20}$$

$$\sum_{k=1}^{D} DD_{kj}(t) \times \sum_{l=1}^{(t-1)} Y_j(l) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.21}$$

$$\sum_{k=1}^{S} SD_{kj}(t) \times \sum_{l=1}^{(t-1)} Y_j(l) = 0, \quad j = 1 \ldots D, t = 1 \ldots T. \tag{9.22}$$

9.1.1 Model complexity

If the model is solved as a multi-stage model, the number of variables in each stage will be $D^2 + 2 \times D + 2 \times D \times S$ with up to $12 \times D + 2 \times S + S \times D + 2$ constraints. The search space in each stage will be approximately $2^{D^2+2\times D+2\times S\times D}$. For example, if we have 200 dams and 10 sires and we would like to optimise for 5 stages, there will be 44,400 variables in each stage with at most 2,422 constraints, and approximately search space size of $10^{13,365}$.

If the model is expanded as a single-stage non-linear binary model, the number of variables will be $T \times D^2 + 2 \times D \times T + 2 \times D \times S \times T$ with $12 \times D \times T + 2 \times S \times T + D \times S \times T + 2 \times T - D$ constraints. The search space will be $2^{T\times D^2+2\times D\times T+2\times D\times D\times T}$. In the previous example, there will be 222,000 variables in all stages with 11,910 constraints, and approximately search space size of 10^{66828}.

9.2 Experimental design and objectives

The experiments' objective (to be presented in the rest of the chapter) is to evaluate different heuristics for mate-selection over 5 stages. It is common practice in animal genetics to simulate a herd with characteristics derived from real life situations. Consequently, we need to simulate a herd that endorses a relatively real life scenario. Therefore, the simulated model incorporates some of the potential aspects of the problem. A more realistic version of the simulation model presented in Section 8.3 is used in this chapter. The differences between the simulation model used for the previous single-stage experiment and the one used for the multi-stage experiment, presented in this chapter, include:

1. The season-year-effect, YS_i, in Equation 8.11 is separated into a year effect, Ye, and a season effect, S_i, in Equation 9.23.

2. The herd mean, M in Equation 9.23, is 5500 to match the latest figures of Australia.

3. To simulate a more realistic situation, two herds were simulated: a nucleus herd for generating AI-sires to be used by a commercial herd.

For the reader's convenience, a summary of the simulation model will follow with the previous modifications. The experimental setup is divided into two parts. First, we need to simulate AI-sires and an initial starting herd. Second, we need to optimise the process of selection and allocation between the cows in this herd and the AI-sires. The experimental design for these two parts are discussed in the following two sub-sections.

9.2.1 The simulation model for the initial herd

Two herds were simulated. The first was used to generate AI-sires for each year for the second herd to use. The following model was used to simulate an Australian Holstein Friesian breed in both herds to generate the initial set of animals. The records were generated by sampling from the following equation.

$$Y_{ijk} = \mu + Ye + S_i + A_j + PE_j + E_{jk} \tag{9.23}$$

where μ is the herd mean, Ye is the year effect, S_i is the season fixed effects where $i = 1, \ldots, 4$, A_j is the additive genetic effect for animal j, PE_j is the permanent environmental effect for animal j, and E_{jk} is the residual effect for the k^{th} record of animal j. Here, we have a single record for each animal.

The heritability (h^2) and repeatability (r) were 0.25 and 0.40 respectively. The herd mean (μ) was 5500. The four season effects were -100, 0, 100, 200. The year effect was sampled using a uniform distribution between 0-200. The phenotypic (σ_P), additive (σ_A), permanent environmental (σ_{PE}), and residual (σ_E) standard deviations were calculated using Equations 8.12-8.15.

The breeding values for the sires and the dams were sampled as mentioned in Section 8.3.1. Each dam was allocated a season effect at random, where the pseudo-random number was sampled from a uniform distribution $U(0, 1)$. The year effect was sampled from $U(0, 200)$ for each year. The permanent environmental and residual effects were sampled from $N(0, \sigma^2_{PE})$ and $N(0, \sigma^2_E)$ respectively. The Mendelian sampling, ϕ, in Equation 8.16, is $N(0, \sigma^2(\phi))$. $\sigma^2(\phi) = 0.5 * \sigma^2_A * (1 - 0.5(F_s + F_d))$, where F_s and F_d are the parents' inbreeding coefficients.

The nucleus herd

A nucleus herd was simulated to generate AI-sires required for breeding commercial herds. To mimic a practical genetic relationship structure, simulation of both a nucleus herd and a commercial herd is required. In year 0, 500 dams and 250 sires were generated independently using the previous model. For each year, the best 10 sires were saved in the AI-sires' list and mated with 100 dams at random. Additionally, 100 sires, not including any AI-sire, and 100 dams were selected at random for culling. The mating ratio between sires and dams was 1:10 and the simulation was carried out for 21 years. Each mating resulted in two progeny, one male and one female, for replacement. The AI-sires' list in each year was saved in a list to be available for mating for the cows in the commercial herd.

The commercial herd

In year 0, 200 dams were simulated using the previous model. The population was mated at random for 20 years. In each year, half of the dams was selected at random for culling and the other half was mated at random with the AI-sires generated previously. One may notice that the number of years for the nucleus herd is 1 year more than the initial herd. The AI-sires generated in the additional year are used for the optimisation model. Each dam selected for mating was assigned an AI-sire at random and the progeny is assumed to be a heifer.

9.2.2 Experimental design for the optimisation model

The experiments to be presented here are very computationally expensive because of the relationship matrix's generation. A complete run of length 30,000 objective-evaluations took around 30 hours on a 400Mhz PC. Two super-computers and 1 Sun-Sparc server were utilised to distribute the experiments. In solving the multi-stage model, it is not practical to wait until the algorithm converges to a solution since the farmer requires to reach a solution within a reasonable time. Consequently, the number of objective function evaluations is used as a criteria to terminate the search. The main objective of this experiment therefore is to select the heuristic that results in the best solution within a maximum of 30,000 objective evaluations. Additionally, the search is

terminated if the algorithm does not improve the best solution found so far within 3,000 objective evaluations. This number is obtained by randomly searching for solutions. It is found, as will be described later in Section 9.4, that the average number of steps needed by random search to stabilise (to reach the best solution found) is less than 3,000 objective evaluations. Therefore, it is decided that an algorithm which does not improve the solution within 3,000 objective evaluations is to be terminated. Both criteria are valid in the literature (Michalewicz and Fogel 2000). The variance of the best solutions found over 10 different runs with different seeds, is used as a measure for the stability of these heuristics.

One nucleus and one commercial herd were simulated using the model discussed in the previous sub-section. The total number of sires and dams was 45 and 1250, respectively, representing the total number of animals required for calculating pedigree information for the herd. The commercial herd contained 200 dams still alive (*ie.* available for mating) and the nucleus herd contained 10 AI-sires. The maximum number of matings allowed per sire was 20, the number of required culling 100, and the total number of required matings 100. Each experiment is repeated ten times with ten different seeds. The same ten seeds are used for all experiments to guarantee a fair comparison among the algorithms since all algorithms will start from the same point in the search space.

In the optimisation model, as virtual matings are being evaluated for the future, we assume for simplicity that the progeny breeding value is half of the parents as in Equation 8.16 but without the Mendelian term. However, in Shepherd and Kinghorn (Shepherd and Kinghorn 1994), a *Look Ahead Mate Selection* (LAMS) algorithm was proposed to predict the outcomes of virtual matings.

9.3 Problem preparation

9.3.1 Representation of the multi-stage solution

In the proposed strategies, a solution is represented using a two-dimensional array where each row represents a single stage. Each cell in each row is associated with a dam, which is available for allocation, as shown in Figure 9.1. It is obvious in this representation that the pedigree

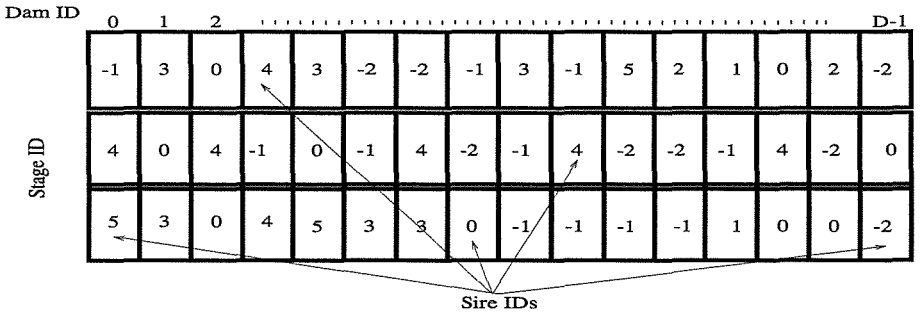

Figure 9.1: The data structure for a solution in the multi-stages model.

information is missing. To illustrate how the pedigree information exists in the proposed representation, consider the value "-1" in the first column and first row. This value entails that the first dam is to be culled in the first stage. The first mating in the first stage is taking place between the second dam and sire number "3". Therefore, the first cell in the second row, which corresponds to the first culled cow from the first stage, corresponds now to the first progeny.

In summary, in stage $t+1$, the progeny of stage $t-1$ take the culled animals' places in stage t in the same order of which the matings in stage $t-1$ and culling in stage t occurred. It is worth mentioning that, which progeny occupy which cell does not affect the solution, since each index in the chromosome has a significant meaning only when it is associated with an animal. Having this representation, the logical constraints connecting the stage with each others are satisfied. Additionally, we do not need to store the pedigree information for all possible solutions, which is not a feasible thing to do, since it can be generated using the heuristic defined above when required. This representation reduces the search space to

$$\begin{pmatrix} T \times D \\ T \times D - C \end{pmatrix} \times S^{(T \times D - C)} \tag{9.24}$$

where T is the number of stages, D the number of dams, S the number of sires, and C the number of culling. When $T = 5$, $D = 200$, $S = 10$, and $C = 100$, the search space is approximately 10^{1000}!

It is important to emphasise here that this representation removes redundancy from the optimisation model without excluding any possible optimal solutions. Therefore, the whole search space of the original model is still preserved in this representation, but in a compact way while it is guaranteed that the optimal solution is reachable by this representation (*ie.* it is one of the

```
function neighbour(x', ζ)
    x ← x'
    neighbour_length = ζ × random()
    foreach row i in x
        for k = 1 to neighbour_length
            j = random() ×x
            x[i][j] = random() × number_of_sires
        next k
    next i
    repair(x)
    return x
end function
```

Figure 9.2: Generation of neighbour solutions.

10^{1000} solutions).

9.3.2 Generation of neighbour solutions

A solution x is generated in the neighbourhood of another solution x' by randomly changing up to ζ cells in each stage of x', where ζ is the maximum neighbourhood length. The neighbourhood length is measured in terms of the number of cells with different values in both solutions, and is equivalent to the hamming distance between both solutions if they were mapped to the mating matrix M. Figure 9.2 presents the algorithm used for generating neighbour solutions. We will reserve the term *neighbourhood size* to represent the number of solutions examined in a neighbourhood. Therefore, a neighbourhood size of 20 requires calling the algorithm in Figure 9.2 20 times.

9.3.3 Constraint satisfaction method

The repair operator is used in all experiments to satisfy the constraint system. The algorithm is similar to the one presented for the single-stage model, Figure 8.3, with the addition of a loop over all stages. It is important to note here that the additional constraints connecting the animals in different stages are satisfied by the solution's representation.

9.3.4 Handling the multi-objective problem

Since this is a multi-objective problem, one of the methods for handling multi-objective problems, discussed in Chapter 6, should be used. Similar to the single-stage model, the weighted-sum method will be used for combining the objectives. However, this is a difficult process when the objectives are from different dimensions. We may assume here that the preferential weights unify the dimensions of different objectives, but the problem of the magnitude of each objective remains. In Chapter 8, we overcame this problem by choosing preferential weights reflecting each objective's magnitude. Therefore, each weight represented the importance of each objective in addition to its magnitude. This might not be a desirable thing to have. To overcome this problem, each objective is divided by a constant representing an estimation of the standard deviation of the values of this objective. Ten runs were undertaken for 200 objective-evaluations each and the standard deviation of each objective was calculated. In all experiments, each objective was scaled by this constant before being evaluated. These constants are 160331 for phenotypic values, 14936.3 for genotype, 29.6864 for inbreeding, and 815.292 for coancestry. The following differential weights were then used: $\alpha = 1$, $\beta = 1$, $\gamma = -1$, and $\delta = -1$ for phenotypic, genotypic, inbreeding, and coancestry respectively. In real life, different weights may be used according to an economic model. In this thesis, we assume that all the weights are equal since changing them will change the values obtained by each heuristic, although it should not change the conclusion in terms of which heuristic is better. All the results are presented after unscaling the objectives. Therefore, while each technique is optimising the problem, each of these objectives have equal influence on the optimisation process. It is important, however, to emphasise that the decision of what is the best set of weights is problem specific and outside the scope of this thesis. This decision needs the employment of economic models for the farm. However, for any set of weights to be significant, the problem of the objectives' magnitude should be solved. Therefore, we emphasise in this thesis the problem of magnitude.

9.4 Experiment 1: Random search

A random search algorithm is used to provide a lower bound on the acceptance of the solutions generated by all other algorithms. This is similar to a mate selection strategy where the farmer

select and mate the animals at random. The algorithm is presented in Figure 9.3. It generates solutions randomly then each solution is introduced to the repair operator for constraint satisfaction. Following the repair, the solution is evaluated by the objective function and if it is found to be better than the present best solution found, it is saved as the new best solution found.

```
function random_search
    Generate x_0 at random
    repair(x_0), f_0 = f(x_0)
    x_opt = x_0, f_opt = f_0
    k = 1
    while k < 30,000 do
        Generate x_k at random
        repair(x_k), f_k = f(x_k)
        if f(x_k) > f(x_opt) then x_opt = x_k, f_opt = f_k
        k = k + 1
    return x_opt, f_opt
end function
```

Figure 9.3: The random search algorithm

The algorithm is run for 30,000 objective-evaluations ten different times with different seed initialisation. The average of the best solutions found for the ten runs was 2,013,620 $\pm$ 23,100. These solutions were found after 2,940 $\pm$ 1,710 objective-evaluations on the average. The best solution among the ten runs was 2,058,400. These values will be used as a lower bound for the acceptance of the heuristics' solutions that will be used in the rest of the chapter to solve the problem.

9.5 Experiment 2: Sequential genetic algorithm

The objective of this experiment is to test the level of interactions among the five stages by optimising each stage independently, then evaluating the resultant solutions. The genetic algorithm approach presented in Chapter 8 is used together with the best set of parameters found in the chapter; that is, one-point crossover with modified tournament selection. The algorithm is run ten different times with different seed initialisations. The average best solutions found for the

```
function hill_climber_search
    Input: ζ
    Generate x_0 at random
    repair(x_0), f_0 = f(x_0)
    x_opt = x_0, f_opt = f_0
    k = 1
    while k < 30,000 do
        Generate x_k ∈ neighbour(x_opt, ζ)
        repair(x_k)
        if f(x_k) > f(x_opt) then x_opt = x_k, f_opt = f_k
        k = k + 1
    return x_opt, f_opt
end function
```

Figure 9.4: The hill climber algorithm

ten runs was 3,429,260 ± 30,500. The best solution among the ten runs was 3,483,700.

9.6 Experiment 3: Greedy hill climber

Methods

A greedy hill climber algorithm is used to solve the problem. The algorithm is presented in Figure 9.4. It generates solutions from the neighbourhood (using the function **neighbour** presented in Figure 9.2 and the function **repair** described in Section 9.3.3) of the best solution found so far. If the resultant solution is better than the best solution found, the new solution becomes the best solution found and the search continues from there; otherwise the new solution is rejected and another one is generated.

The algorithm is run for 30,000 objective-evaluations ten different times with different seed initialisation. The run is terminated if 3,000 objective-evaluations elapse without an improvement in the best solution found. Five neighbourhood lengths are tried; 100%, 50%, 10%, 5%, and 1% of the chromosome length.

Results and discussion

The results of the hill climber algorithm are presented in Table 9.1. A general trend can be seen in the table between the neighbourhood length and the quality of the solution obtained. The smaller the neighbourhood length, the better the solution. The best solution found corresponds to neighbourhood length of 1% of the chromosome's length (a change of 2 cells). We may note that a neighbourhood length of 100% is not equivalent to random search because the neighbourhood length represents the maximum number of changes in the chromosome and not the exact number.

Table 9.1: The greedy hill cilmber results with different five neighbourhood lengths.

Neighbourhood length	average fitness	average # objective-evaluations	Best solution
100%	2,754,550 ± 83,000	27,740 ± 4,380	2,834,700
50%	2,914,290 ± 25,200	28,950 ± 1,530	2,956,700
10%	3,284,230 ± 25,200	29,800 ± 240	3,320,300
5%	3,430,310 ± 21,000	29,840 ± 130	3,469,400
1%	3,510,180 ± 15,800	29,600 ± 350	3,533,000

9.7 Experiment 4: Simulated annealing

Methods

A homogeneous simulated annealing algorithm is employed in this strategy and is shown in Figure 9.5. The algorithm starts with two inputs from the user, the initial temperature T, and the neighbourhood length ζ. The initial chain length L is set to 1000 and the number of coolings C to 100. This setup, together with a decrement in the chain length of 0.968, guarantees a maximum number of objective evaluations of 30,000. The temperature is decremented by a constant equal to the initial temperature divided by the total number of coolings.

To gain an insight about an appropriate value for the initial temperature, 10 runs of length 200 objective evaluations were made. It was found that 99% of the solutions can be accepted with average temperature of 90 ± 4. Consequently, four initial temperature levels (100, 50, 10,

```
function SA
    Input: ζ and T
    C = 100, L = 1000, i = 0
    Generate x_0 at random
    repair (x_0), f_0 ← evaluate x_0
    initialise best solution found x_opt to be x_0 and its objective value f_opt = f_0
    initialise current solution x_current to be x_0 and its objective value f_current = f_0
    temperature_step = T/C
    for k = 0 to C
        for j = 0 to L
            i = i + 1
            x_i ∈ neighbour(x_current, ζ), f_i ← evaluate x_i
            Δ(f) = f_i − f_current
            if f_i > f_opt then x_opt = x_i, f_opt = f_i
            if f_i > f_current then x_current = x_i, f_current = f_i
            else if exp(Δ(f)/T) > random (0,1) then x_current := x_i, f_current = f_i
            if last update of x_opt > 3,000 exit for
        next j
        T = T− temperature_step
        L = L * 0.968
        if last update of x_opt > 3,000 exit for
    next k
    return x_opt and f_opt
end function
```

Figure 9.5: A homogeneous simulated annealing algorithm for the multi-stage model.

and 1) are experimented with against three different neighbourhood lengths, 10%, 5%, and 1% of the chromosome length. Therefore, a total of twelve experiments is carried out, with each experiment runs ten different times with different seeds while the same ten different seeds were fixed among all experiments. A maximum of 30,000 objective evaluations were set on each run with a stop occurring either when this maximum is reached, or when 3,000 objective evaluations elapse without an improvement in the best solution found.

Results and discussion

The algorithm behaved like random search at high temperature levels; 100 and 50. The reason for this is that the algorithm terminated while the temperature level was still very high because of the condition of an improvement in the best solution found within 3,000 objective evaluations. Therefore, only the results at temperature levels 10 and 1 are presented in Table 9.2. The best performance of SA (in terms of the best solution found) in this experiment occurs with a temperature level 1 and neighbourhood length of 5%.

Table 9.2: Simulated annealing results at temperature levels 10 and 1 respectively.

	Neighbourhood length	average fitness	average # objective-evaluations	Best solution
Temperature = 10				
	10%	$2,032,540 \pm 24,200$	$2,220 \pm 1,740$	2,063,600
	5%	$2,042,000 \pm 20,000$	$3,420 \pm 2,060$	2,068,400
	1%	$1,976,840 \pm 16,800$	$2,710 \pm 1,410$	2,000,200
Temperature = 1				
	10%	$2,404,580 \pm 41,000$	$2,730 \pm 1,870$	2,474,600
	5%	$2,407,730 \pm 34,700$	$2,370 \pm 950$	2,493,000
	1%	$2,419,290 \pm 36,800$	$2,550 \pm 1760$	2,469,700

9.8 Experiment 5: Ant colony optimisation

Methods

To describe any ant system for combinatorial optimisation problems, Bonabeau et al. (1999) require the definition of five components:-

1. **Problem representation**

   A graph representation inherently exists in the problem. Due to the dynamic nature of the problem, it might be difficult to imagine this graph. We have three dimensions in each solution - dams, sires, and time. If we fix the time dimension (*ie.* a single-stage problem), the problem is a transportation model and can be expanded as an assignment model. A set of nodes representing the dams are fully connected to a different set of nodes representing the sires. A path is defined by starting from one dam, moving to a sire, moving to a different dam, and so on. The goal is to step over all the nodes for the dams while satisfying the other constraints.

Now, let us add the third dimension; the time. Actually, in every stage, the previous definition of a graph is preserved. But how do we connect the stages together? The additional nodes at stage $t+1$ depend on the visited arcs in stage t (A female node in stage $t+1$ is the daughter resulted from an allocation of a sire to a dam - visiting the arc connecting this sire and that dam - in stage t). This is very interesting since the graph structure is dynamic, and varies according to the visited arcs in each stage.

2. **Heuristic desirability**

The ACO strategy adopted here is similar to the MMAS-QAP (Stutzle 1998), where no heuristic information is used. Therefore, the pheromone is deposited as presented in Equation 6.11.

3. **Constraint satisfaction method**

Two constraint satisfaction methods are implemented. The first uses the repair operator previously mentioned in Section 9.3.3 (see Figure 8.3). The second is a constructive heuristic for building up the solution. The constructive algorithm is given in Figure 9.6.

The constructive algorithm builds up a solution using the probabilistic choice rule while maintaining the feasibility of the chromosome. It starts with assigning the dams in each stage to culling with a probability proportional to the amount of the pheromone allocated to the culling decision of this dam. After satisfying the culling constraint, the same process is repeated to satisfy the number of mating required. We may recall that culling is represented with a dummy sire in the pheromone matrix. Therefore, mating decisions are undertaken in the same way as culling decisions.

4. **Pheromone updating rule**

Two pheromone update rules are used. One does not use pheromone evaporation while

```
procedure constructive(x')
    foreach stage g
        while Cull ≠ number_of_allowed_culling do
            randomly select dam j
                if j is not being allocated then
                    if j passed the probabilistic choice rule then
                        assign j to culling, Cull = Cull + 1
        while Mat ≠ number_of_allowed_matings do
            randomly select dam j
                if j is not being allocated then
                    randomly select sire i
                    if alloc_i ≠ maximum_number_of_sire_allocations then
                        if j and i passed the probabilistic choice rule then
                            assign i to j, Mat = Mat + 1, add 1 to alloc_i
end procedure
```

Figure 9.6: The constructive algorithm for ACO

the other does. The two rules are given by Equation 6.15. Pheromone evaporation occurs when $\rho < 1$. In each case, four different ways for calculating $\Delta_{ij}\tau^k(t-1)$ are implemented. These are:

(a) The pheromone is updated only with the reciprocal of the objective value corresponding to the best ant, Equation 6.16 (call it *best*)

(b) The pheromone is updated with the total fitness of the ants visited the arc ij, where the fitness is defined using a linear normalisation of the objective value corresponding to the ant, divided by the total objective values achieved by all the ants in the same iteration, (call it *fitness*)

$$\Delta\tau_{ij}^k(t-1) = \begin{cases} \frac{\sum_{k\in K} J^k}{\sum_{l\in L} J^l}, & \text{if dam } i \text{ is allocated to sire } j \text{ in stage } t \\ 0 & \text{otherwise} \end{cases} \tag{9.25}$$

where K is the set of ants visited ij, L is all the ants in the iteration, and J^k is the solution's objective value found by ant k.

(c) The pheromone is updated only with a constant taken to be 0.1 in our implementation (call it *constant*)

$$\Delta\tau_{ij}^{k}(t-1) = \begin{cases} K \times \alpha & \text{if dam } i \text{ is allocated to sire } j \text{ in stage } t \\ 0 & \text{otherwise} \end{cases} \tag{9.26}$$

where, K is the number of ants visited ij at iteration t.

(d) The pheromone is updated only with the reciprocal of the objective value corresponding to all ants, Equation 6.16, where C in the equation is taken to be 1000 in our implementation. (call it *objective*)

5. **A probabilistic transition rule**

   The ACO probabilistic transition rule adopted here is similar to the MMAS-QAP (Stutzle 1998) and is given by Equation 6.11.

After constructing a solution, each ant applies the local search algorithm to improve its current solution. The new improved solution, if it exists, replaces the ant's original solution. The number of trials the ant attempts to improve is the neighbourhood size to be searched for this ant. A population of 1 and 5 ants were experimented with. The use of a single ant is similar to the FANT algorithm (Taillard 1998). To limit the maximum total number of objective evaluations to 30,000, the following equation should hold

$$number\ of\ ants \times the\ neighbourhood\ size \times the\ number\ of\ iterations = 30,000$$

Three neighbourhood sizes are tried: 50, 100, 150 for 1 ant and 10, 20, 30 for 5 ants. To see the impact of neighbourhood size, the number of ants $\times$ the neighbourhood size is fixed (50×1 corresponds to 10×5, 100×1 corresponds to 20×5, and 150×1 corresponds to 30×5). Therefore, 96 experiments are carried out (each experiment is run 10 times with different seeds) to find the best combination of parameters which will result in the best solution.

Results and discussion

The central focus of the experimental design aims to compare the appropriateness of four configurations:

Table 9.3: Relationship between the number of ants and neighbourhood length.

	a single ant Neighbourhood Size		
	50	100	150
Avg best solutions	2,097,990 ± 68,300	2,168,620 ± 94,900	2,314,360 ± 32,100
# of objective-evaluations	2,420 ± 2,010.0	2,330 ± 1,920.0	2,650 ± 2,090.0
Best solution found	2,229,500	2,346,700	2,414,900
	five ants Neighbourhood Size		
	10	20	30
Avg best solutions	2,033,640 ± 28,000	2,076,690 ± 24,100	2,111,680 ± 25,900
# of objective-evaluations	2,590 ± 1,970.0	2,430 ± 2,010.0	2,700 ± 1,860.0
Best solution found	2,128,900	2,153,700	2,194,000

- fewer ants and longer neighbourhood length vs more ants with shorter neighbourhood length,
- constructive algorithms vs repair operator,
- with pheromone evaporation vs without pheromone evaporation, and
- the four pheromone update rule.

Fewer ants/longer neighbourhood vs more ants/shorter neighbourhood

In this section, the results for the 96 experiments are grouped according to the number of ants and the neighbourhood size. The key question here is: are fewer ants with longer neighbourhood search better than more ants with shorter neighbourhood search? This question can be restated in a different, still equivalent, way: where does the real improvement in the ants algorithm come from, the ants or the local search technique?

In Table 9.3, the best performance occurred with a single ant and neighbourhood size of 150 but the differences are not statistically significant. This result may suggest that longer neighbourhood size has more influence than the number of ants used. ACO algorithms suffer from a severe scalability problem (Dorigo and Caro 1999). This may seem to be the reason behind the influence of the neighbourhood size in our problem.

Table 9.4: Comparing ACO with constructive algorithms against the repair operator

	Constructive algorithm	Repair operator
Avg best solutions	2,138,440 ± 111,600	2,129,550 ± 97,100
# of objective-evaluations	2,630 ± 1,990.0	2,410 ± 1,960.0
Best solution found	2,414,900	2,387,600

Table 9.5: Comparing ACO with/without pheromone evaporation

	With pheromone evaporation	Without pheromone evaporation
Avg best solutions	2,157,770 ± 105,400	2,110,510 ± 98,600
# of objective-evaluations	2,430 ± 2,020.0	2,610 ± 1,930.0
Best solution found	2,414,900	2,387,600

Constructive algorithm vs repair operator

In this section, the results for the 96 experiments are grouped according to the means of creating a step in the local search. The first means is the constructive algorithm presented in the previous section. The second is randomly then repairing the resultant solution. The crucial point here is to answer the question: does the constructive algorithm, which uses the ants routing table, improve the solutions generated within the neighbourhood?

In Table 9.4, the constructive algorithm performed better than the repair operator but the differences are not statistically significant. This result entails that the constructive algorithm has a positive bias (*ie.* a bias which helps in improving the solution), an important characteristic in large search spaces.

With/without pheromone evaporation

In this section, the results for the 96 experiments are grouped according to whether or not pheromone evaporation is used. The fundamental issue here is to answer the question: does pheromone evaporation help in this problem?

In Table 9.5, the best performance occurred with pheromone evaporation but the differences are

Table 9.6: Comparing the ant algorithms with four different pheromone update rules.

	best	*fitness*
Avg best solutions	2,139,090 ± 103,800	2,131,710 ± 100,900
# of objective-evaluations	2,590 ± 2,010.0	2,480 ± 2,040.0
Best solution found	2,414,900	2,387,600
	objective	*constant*
Avg best solutions	2,137,520 ± 105,400	2,127,710 ± 108,600
# of objective-evaluations	2,620 ± 1,940.0	2,380 ± 1,920.0
Best solution found	2,414,900	2,371,100

not statistically significant. Therefore, pheromone evaporation helped to improve the solutions' quality.

Pheromone update rule

In this section, the results for the 96 experiments are grouped according to the pheromone update rule. The four pheromone update rules are: *best*, *fitness*, *objective*, and *constant*. The first (*best*) and third (*objective*) rules are extracted from the literature as pointed in the previous section. The second (*fitness*) and fourth (*constant*) are proposed here. *fitness* pheromone update rule measures the value of adding the concept of competition between the ants through adjusting the pheromone update matrix by the fitness of each. *constant* reverse this impact and simply looks at all ants as if they are similar.

In Table 9.6, it is found that both *best* and *objective* succeeded to find the best solution but the differences are not statistically significant. However, *best* was better (although statistically not significant) in terms of the average of the ten runs, their standard deviations, and the number of objective-evaluations.

Summary of ACO results

Although individually they were statistically indifferent, overall, the best performance of the ACO algorithm occurred with one ant, a neighbourhood size of 150 using the constructive algorithm with pheromone evaporation and either the *best* or *objective* pheromone update rule. However, it is worth noting that SA produced better results than the ACO. SA found a better best solution

and better average best solution with less standard deviations. This does not mean that ACO is not suitable, but it does have a scalability problem. This issue will be further investigated in the conclusion of the chapter.

9.9 Experiment 6: Markov chain tabu-search (a new algorithm)

Methods

Paulli (1993) found that the choice of the tabu-list's size has a large influence on the solution's quality and it varies considerably among problems. Furthermore, he claimed that SA is much better than TS for the quadratic assignment problem. Recalling from the previous chapter that the single-stage problem is a quadratic transportation model, and the multi-stage model discussed in the current chapter is a dynamic transportation model, this gives an expected bad performance for tabu search. The side-effects of the tabu-list's size has been discussed in Chapter 6.

The previous points motivated the development of a new version of TS which we called *markov chain tabu search* (MCTS). Here, the tabu-list will be referred to as the *probabilistic tabu-list* (PTL). There is almost no relation between MCTS as presented here and a version of tabu search called *probabilistic tabu search* (PTS) (Laguna 1997). Glover and Manuel (1997) list PTS under neglected tabu search strategies. In the end of this section, we will present the differences between MCTS and PTS. In MCTS, the PTL's size is always fixed and the structure depends on the representation. For example, in our problem a solution is represented using a two-dimensional array where one dimension, t, represents the number of stages and the second dimension, j, represents the dams. The PTL is represented using a three-dimensional array where in addition to the two-dimensional solution array, a third dimension, i, is added of size equal to the number of sires. Each cell in the three-dimensional array represents the probability that sire i is to be allocated to dam j in stage t. If we refer to this probability as π_{tij}, then the following conventional probability conditions should be satisfied all the time:

$$0 \leq \pi_{tij} \leq 1 \tag{9.27}$$

$$\sum_{i=1}^{S+1} \pi_{tij} = 1 \tag{9.28}$$

where S is the number of sires. The matrix is initialised with all values equal to $\frac{1}{S+1}$. The reward/penalty is initialised with 1% of the initial value used in the PTL; that is, $\frac{1}{100\times(S+1)}$. The algorithm is depicted in Figure 9.7. It is worth noting that this algorithm is different from the *Penalty* search version of tabu search (Shivastava and Chen 1993), as we always center the neighbourhood search over the best-solution found so far, whereas the penalty search version of tabu search does not.

One may ask if this is still a tabu search algorithm, although we do not have an explicit tabu list. The answer is simply yes. Since the elements in the PTL matrix can reach the threshold, and therefore are tabu, the definition of "tabu" is still preserved in the PTL matrix.

Every time the MCTS algorithm selects a new solution from the neighbourhood, a reward and/or a penalty is assigned to each cell in the PTL which is present in the solution. If the new solution is better than the previous best solution found, the assignments corresponding to the previous best solution found are penalised and those corresponding to the new solution are rewarded. That is, if sire 5 is allocated to dam 3 in stage 1 in the previous best solution found, the cell which corresponds to sire 5, stage 1, and dam 3 in the PTL is decreased by a constant. If the previous best solution found is still better than the new solution, the best solution found is rewarded and the new solution is penalised. Therefore, the algorithm uses a double re-inforcement approach. In this way, instead of storing the set of directions which are tabu, they are indirectly penalised in the probabilistic tabu-list. The algorithm is based on Markov chain since each new PTL depends only on the previous one and represents a transition matrix between states. The update rule can be represented as a transition matrix as well, with all cells equal to 0 except those needing to be rewarded or penalised, which they are set to the penalty/reward constant. Note that keeping rewarding the best solution found as long as it does not change, helps to speed up the algorithm, although it may cause stagnation which will be overcome as will be explained in the discussion of the function *choose*. Speeding up the algorithm is a necessity for two reasons:

```
procedure MCTS
    Input: ζ
    initialise discount step (reward/penalty term) to be 1/(100×(S+1))
    generate π^0 with π^0_tij = 1/(S+1)
    generate solution array x^0 at random
    repair(x^0)
    f^0 ← evaluate x^0
    x^opt ← x^0 and f^opt ← f^0
    k = 1
    while M < maximum number of objective-evaluations
       x^k ← choose(x^opt, π^{k-1})
       repair(x^k)
       f^k ← evaluate x^k
       M = M + 1
       for l := 1 to Neighbourhood size
          x^k_new ← neighbour(x^k, ζ)
          repair(x^k_new)
          f^k_new ← evaluate x^k_new, M = M + 1
          if f^k_new > f^opt, then f^opt ← f^k_new, x^opt ← x^k_new
          if f^k_new > f^k, then f^k ← f^k_new, x^k ← x^k_new
       if f^k > f^opt, then
          f^opt ← f^k, x^opt ← x^k
          foreach stage t
             foreach cow j
                add discount step to π^{k-1}_tij where i = x^k_tj
                subtract discount step from π^{k-1}_tij where i = x^opt_tj
       else
          foreach stage t
             foreach cow j
                add discount step to π^{k-1}_tij where i = x^opt_tj
                subtract discount step from π^{k-1}_tij where i = x^k_tj
       π^k ← π^{k-1}
    k = k + 1
end procedure
```

Figure 9.7: The Markov chain tabu search algorithm.

1. Markov chain based search techniques are very slow by nature and it can take a very long time to reach equilibrium.

2. The greediness of the algorithm is overcome by the repair operator which introduces disruption to the neighbourhood and therefore a probability to escape local optima.

There remains a question here, how does the MCTS algorithm choose x^k using π^{k-1}; that is, the function *choose*(x^{opt}, π^{k-1}). The algorithm for this function is shown in Figure 9.8.

In Figure 9.8, the parameter α represents the threshold of rejecting the allocation of sire i to dam j. Now, let us assume that the initial probability for all sires was 0.1, $\alpha = 0.05$, the discount

```
function choose(x^opt, π^{k-1})
    x' ← x^opt
    foreach stage t
        randomly select J < number of dams
        for j = 1 to J
            randomly select sire i
                if π_tij > α then
                    x'_tj = i
    return x'
end function
```

Figure 9.8: The generation of neighbourhood solutions in the MCTS algorithm.

step = 0.01, the solution did not improve after 5 objective-evaluations from the start, and sire i was allocated to dam j in all last 5 stages. Therefore, $\pi^5_{tij} = 0.05$ since we kept penalising the probability. The algorithm illustrated in Figure 9.8 will force dam j to be allocated to a different sire. The question is, can sire i be allocated later on to dam j? The answer is yes, since the repair operator does not see the probability matrix π; therefore, even though that it is decided by the probability matrix that this sire is tabu, the repair operator introduces some distortion to the influence of the probability matrix.

To guarantee that the algorithm will not stagnate at some point (*ie.* a sire is always allocated to the same dam), we need to choose the value of α carefully. Assume that we need to run the algorithm for up to 1,000 objective-evaluations; the initial probability is 0.1, the discount factor is 0.01, $\alpha = 0.05$, and we have 10 sires (including a dummy sire for culling). In this case, after around 45 objective-evaluations without an improvement in the best solution found, there is a possibility that the algorithm will keep on this sire for this dam forever. We need to avoid stagnation if this occurs to all dams in the solution. Note that the solution does not change and the repair operator has no effect since the solution is still feasible. The obvious way to overcome this, is to add the discount factor every some number of objective-evaluations to those cells in the probability matrix which reached the minimum rejection level α. This would force the algorithm to change the current solution and escape the current local optimum.

It is important to mention here that the algorithm differs from any tabu search since it starts all the time from the best solution found (the input to the function *choose*(x^{opt}, π^{k-1})). This may imply that this algorithm is a greedy algorithm. However, this is not the case because the

neighbourhood of the step generated by the function *choose* is searched regardless of whether this step generated a better solution than the best found so far or not. Also, every point in the search space is reachable from the best solution found (see the fourth line in the function *choose*). We can imagine the algorithm as a search technique which starts with the best solution found and try to take steps in the space to find a better neighbourhood, while these steps themselves may downgrade the best solution found. The differences between the MCTS and PTS are:

- In essence, PTS is a hybrid of simulated annealing and tabu search. It is considered as a generalisation of tabu search through the use of a simulated annealing approach to decide on the acceptance of a move. MCTS is a reinforcement approach to tabu search. It does not use the probability matrix to accept or reject a solution, but to generate a solution.
- In PTS, the next step is always accepted, while in MCTS the next step within the neighbourhood is always accepted within the neighbourhood but it is not accepted to change the current neighbourhood's centre unless it improves it.
- In PTS, the probability matrix represents the transition probability from a solution to another, while in MCTS the probability matrix represents the transition probability of each variable in the problem.
- In PTS, a new solution is generated within the neighbourhood based on the probability matrix. In MCTS, a new solution is generated from the best solution found so far using the probability matrix and a step within the neighbourhood is generated regardless of the probability matrix.
- In PTS, the probability matrix is updated based on the evaluation of the solution, whereas in MCTS the probability matrix is updated using a constant.
- In PTS, a solution is accepted based on the probability matrix using the relative probabilities, whereas in MCTS a solution is generated from the probability matrix using a threshold function.

Results and discussion

The three parameters that we may need to determine in the MCTS algorithm are: the rejection level, the neighbourhood size, and neighbourhood length. We keep the discount factor constant

- since it is correlated to the rejection level - and change the rejection level instead. The initial probability is $1/11 \approx 0.091$ for each cell in the probability matrix, the discount factor is taken to be 0.001, and $\alpha \in \{0.02, 0.05, 0.08, 0.09\}$. Every 100 objective-evaluations, the discount factor is added to random number of elements in the matrix reached the rejection level and subtracted from random number of elements in the matrix exceeding the rejection level. Six neighbourhood sizes of 150, 100, 50, 10, 5, and 1 and neighbourhood lengths of 10%, 5%, and 1% were tested as shown in Table 9.7. A neighbourhood size of 1 means that the algorithm is one-step look ahead algorithm.

In Table 9.7, the best combination is found with the shortest neighbourhood size (1), the shortest neighbourhood length (1% of the chromosome size or equivalently 2 cells for each stage), and the highest rejection level (0.09). On the contrary to ACO, a shorter neighbourhood size is better in MCTS. Generally, MCTS outperformed the four previous techniques.

The previous results need further explanation. We may notice that there is a relation between the neighbourhood size and the number of points visited in the space. With a large neighbourhood size, the algorithm spends most of the time in exploring the neighbourhood (intensification of local search) while reducing the exploration of the overall search space (sacrificing with diversification of global search) because the number of objective evaluations is fixed. With a small neighbourhood size, the reverse is occurring. The probability matrix is different. Continuous update of the probability matrix emphasises the exploration of the overall search space (intensification of global search). Therefore, the results found here suggest that the intensification of the search while globally exploring the search space through the probability matrix is more beneficial than the local intensification of the search through the neighbourhood. This result is consistant with the fact that the search space is huge; therefore, spending time in the neighbourhood may not be a good idea.

Table 9.7: The results for the Markov chain tabu search method.

			Neighbourhood Size		
α	ζ		150	100	50
0.02	10%	Avg best solutions	2,357,290 ± 28,400	2,323,650 ± 21,000	2,277,410 ± 22
		# of obj-evaluations	3,220 ± 1,630	3,100 ± 2,190	3,770 ± 2,1(
		Best solution found	2,397,500	2,352,200	2,310,100
0.05	10%	Avg best solutions	2,358,340 ± 33,600	2,316,300 ± 24,200	2,299,480 ± 8(
		# of obj-evaluations	3,450 ± 1,800	2,390 ± 1,140	5,520 ± 5,9·
		Best solution found	2,425,600	2,352,200	2,485,700
0.08	10%	Avg best solutions	2,370,950 ± 36,800	2,345,720 ± 68,300	2,523,340 ± 13
		# of obj-evaluations	3,200 ± 1,900	4,130 ± 6,640	15,870 ± 9,2
		Best solution found	2,445,900	2,535,400	2,690,800
0.09	10%	Avg best solutions	2,408,780 ± 46,200	2,462,380 ± 82,000	2,535,950 ± 7(
		# of obj-evaluations	4,040 ± 2,490	9,910 ± 5,630	13,690 ± 6,9
		Best solution found	2,482,000	2,561,500	2,724,600
0.02	5%	Avg best solutions	2,453,970 ± 30,500	2,399,320 ± 33,600	2,329,960 ± 31
		# of obj-evaluations	2,830 ± 1,510	2,820 ± 1,490	4,150 ± 3,0·
		Best solution found	2,489,600	2,444,000	2,382,200
0.05	5%	Avg best solutions	2,456,070 ± 32,600	2,388,810 ± 37,800	2,358,340 ± 10·
		# of obj-evaluations	2,980 ± 1,900	2,170 ± 1,830	5,800 ± 7,0(
		Best solution found	2,501,600	2,444,000	2,646,400
0.08	5%	Avg best solutions	2,461,330 ± 44,100	2,418,240 ± 80,900	2,633,690 ± 12·
		# of obj-evaluations	4,040 ± 2,210	5,200 ± 5,970	15,560 ± 8,0
		Best solution found	2,520,800	2,562,200	2,806,100
0.09	5%	Avg best solutions	2,531,740 ± 82,000	2,605,310 ± 132,400	2,754,550 ± 8(
		# of obj-evaluations	10,090 ± 9,260	12,600 ± 7960	20,260 ± 7,1
		Best solution found	2,653,100	2,735,000	2,891,800
0.02	1%	Avg best solutions	2,439,260 ± 44,100	2,326,810 ± 46,200	2,256,390 ± 43
		# of obj-evaluations	4,740 ± 2,310	4,030 ± 2,900	4,930 ± 2,7(
		Best solution found	2,517,900	2,395,000	2,312,900
0.05	1%	Avg best solutions	2,436,110 ± 43,100	2,337,320 ± 43,100	2,287,920 ± 17(
		# of obj-evaluations	4,350 ± 2,020	3,200 ± 1,820	6,040 ± 7,0(
		Best solution found	2,503,100	2,395,000	2,747,200
0.08	1%	Avg best solutions	2,459,230 ± 76,700	2,616,870 ± 252,200	2,948,970 ± 47
		# of obj-evaluations	5,150 ± 4,340	13,220 ± 10,580	28,680 ± 1,5
		Best solution found	2,607,700	2,953,400	3,021,400
0.09	1%	Avg best solutions	2,800,790 ± 288,000	3,033,050 ± 33,600	3,068,780 ± 98
		# of obj-evaluations	16,740 ± 12,600	27,050 ± 3,620	25,410 ± 6,6
		Best solution found	3,085,000	3,087,400	3,158,100

α	ζ		Neighbourhood Size		
			10	5	1
0.02	10%	Avg best solutions	2,837,570 ± 45,200	3,139,190 ± 56,800	3,293,680 ± 82,000
		# of obj-evaluations	29,760 ± 120	29,760 ± 140	20,850 ± 2,310
		Best solution found	2,887,200	3,212,900	3,386,800
0.05	10%	Avg best solutions	2,948,970 ± 65,200	3,260,050 ± 58,900	3,190,690 ± 70,400
		# of obj-evaluations	28,540 ± 3,940	29,930 ± 50	15,890 ± 2,390
		Best solution found	3,011,100	3,346,700	3,338,500
0.08	10%	Avg best solutions	3,156,010 ± 46,200	3,151,810 ± 88,300	3,050,910 ± 46,200
		# of obj-evaluations	29,920 ± 100	24,620 ± 3,190	7,590 ± 2,030
		Best solution found	3,263,300	3,265,000	3,123,300
0.09	10%	Avg best solutions	3,152,860 ± 45,200	3,091,900 ± 36,800	2,962,630 ± 74,600
		# of obj-evaluations	28,780 ± 1,510	16,290 ± 2,610	5,010 ± 1,610
		Best solution found	3,219,700	3,155,100	3,063,700
0.02	5%	Avg best solutions	2,869,100 ± 63,100	3,195,950 ± 30,500	3,369,350 ± 86,200
		# of obj-evaluations	28,250 ± 3,460	29,710 ± 250	26,030 ± 3,860
		Best solution found	2,947,600	3,269,500	3,498,700
0.05	5%	Avg best solutions	3,012,030 ± 41,000	3,118,170 ± 88,300	3,345,180 ± 72,500
		# of obj-evaluations	29,640 ± 460	29,880 ± 100	23,300 ± 6,310
		Best solution found	3,067,100	3,346,100	3,442,000
0.08	5%	Avg best solutions	3,267,410 ± 33,600	3,332,570 ± 50,400	3,340,980 ± 53600
		# of obj-evaluations	29,940 ± 50	29500 ± 720	22,590 ± 4,210
		Best solution found	3,324,000	3,436,300	3,436,300
0.09	5%	Avg best solutions	3,356,740 ± 39,900	3,360,940 ± 38,900	3,274,770 ± 87200
		# of obj-evaluations	29,880 ± 170	26,440 ± 4,290	17,140 ± 8,740
		Best solution found	3,415,300	3,409,500	3,397,700
0.02	1%	Avg best solutions	2,998,370 ± 42,000	3,263,210 ± 39,900	3,642,600 ± 147,100
		# of obj-evaluations	29,410 ± 730	29,780 ± 190	27,630 ± 7,450
		Best solution found	3,064,500	3,320,800	3,715,300
0.05	1%	Avg best solutions	3,148,650 ± 33,600	3,463,940 ± 31,500	3,737,190 ± 14,700
		# of obj-evaluations	29,530 ± 540	29,860 ± 120	29,990 ± 10
		Best solution found	3,209,500	3,505,100	3,756,700
0.08	1%	Avg best solutions	3,489,160 ± 27,300	3,703,550 ± 23,100	3,800,240 ± 10,500
		# of obj-evaluations	29,930 ± 60	29,920 ± 110	29,970 ± 40
		Best solution found	3,537,500	3,744,100	3,815,800
0.09	1%	Avg best solutions	3,659,410 ± 22,100	3,767,660 ± 12,600	3,805,500 ± 13,700
		# of obj-evaluations	29,950 ± 30	29,970 ± 30	29,910 ± 110
		Best solution found	3,680,100	3,782,700	3,824,600

9.10 Experiment 7: Genetic algorithms

Methods

This strategy employs a GA approach for the multi-stage problem. A chromosome in the multi-stage problem has two dimensions. Therefore, for one and two point crossover operators, the crossover point is calculated for each stage independently from the others. If we have two stages, the crossover point for the first stage may be different from the second stage. Apart from this, all other operators are working in the same way presented in Chapter 6.

Results and discussion

Results for five population sizes are presented in Table 9.8 for population size 30, Table 9.9 for population size 40, Table 9.10 for population size 50, Table 9.11 for population size 60, and Table 9.12 for population size 70. When the population size was 70, the performance declined. To be more confident that the solution did not improve after that, a population size of 100 was tried, but the performance was downgraded again, therefore suggesting that the best population size is 60 under the current experimental configurations.

For population sizes 40, 50, and 60; that is, Tables 9.9, 9.10, and 9.11, a consistent phenomenon is that 1-point crossover with modified tournament reproduction strategy resulted in the best performance overall although it is not statistically significant with respect to 2-points crossover. With population size 30, the uniform crossover operator performed the best with modified tournament, suggesting that with small population size, it had better effect as shown in Table 9.8. With population size of 70, Table 9.12, the two-point crossover operator outperformed the one-point crossover operator although it was worse than that with population size of 60. The best population size which gives the best results based on the setup of these experiments is found to be 60. Surprisingly, gene-based crossover was the worst in the three reproduction strategies. This is not consistent with the results for the single-stage model and may suggest that the interaction between the stages downgraded the performance of the gene-based crossover operator. A consistent trend in all GA experiments is that modified tournament was better than the other two selection strategies for all crossover operators except gene-based crossover. Therefore,

it may suggest that the influence of the selection pressure resulted from the modified tournament strategy is somewhat reversed by the bias introduced by the gene-based crossover operator. The results of this experiment outperformed all previous results except MCTS. The best solution was found with population size 60, 1-point crossover, and modified tournament (Table 9.11).

In Figure 9.9, the performance of the 1-point crossover operator is depicted against the population size using the three selection strategies. The fitness proportion selection strategy is clearly outperformed by the other two while the modified tournament strategy outperformed the other two strategies in all population sizes.

Table 9.8: Genetic algorithms performance on the multi-stage model with population size 30.

The average of the best solutions found over ten different runs with different seeds for the population ± the standard deviation.

Crossover operator	Selection operator		
	Fitness Proportion	Stochastic Baker	Modified Tournament
1-point Avg best solutions	2,497,060 ± 58,900	3,016,230 ± 87,200	3,163,370 ± 78,800
1-point # of objective-evaluations	15,920 ± 5,370	29,130 ± 1,270	8,220 ± 1,330
1-point Best solution found	2,565,900	3,141,500	3,276,900
2-point Avg best solutions	2,606360 ± 44,100	2,852,280 ± 116,700	3,116,070 ± 136,600
2-point # of objective-evaluations	23,810 ± 5,450	20,100 ± 4,250	6,920 ± 1,770
2-point Best solution found	2,670,700	3,031,300	3,290,400
uniform Avg best solutions	2,386,710 ± 39,900	3,136,040 ± 59,900	3,509,130 ± 52,500
uniform # of objective-evaluations	9,510 ± 2,750	29,500 ± 520	28,470 ± 2,940
uniform Best solution found	2,474,900	3,221,400	3,567,000
gene-based Avg best solutions	2,017,830 ± 78,800	1,935,850 ± 25,200	1,923,240 ± 49,400
gene-based # of objective-evaluations	2,950 ± 2,070	1,280 ± 920	180 ± 130
gene-based Best solution found	2,153,800	1,977,500	1,996,400

Table 9.9: Genetic algorithms performance on the multi-stage model with population size 40.

Crossover operator	Selection operator		
	Fitness Proportion	Stochastic Baker	Modified Tourname
1-point Avg best solutions	2,383,560 ± 68,300	2,973,140 ± 78,800	3,349,380 ± 80,90(
1-point # of objective-evaluations	15,080 ± 5,100	29,820 ± 100	12,900 ± 2,380
1-point Best solution found	2,463,300	3,082,000	3,498,400
2-point Avg best solutions	2,440,310 ± 90,400	2,884,860 ± 72,500	3,344,130 ± 56,80(
2-point # of objective-evaluations	17,820 ± 7,650	29,050 ± 1,370	12,200 ± 1,290
2-point Best solution found	2,602,300	2,976,300	3,447,000
uniform Avg best solutions	2,279,510 ± 55,700	2,840,720 ± 76,700	3,252,700 ± 59,90(
uniform # of objective-evaluations	8,120 ± 2,760	26,620 ± 4,320	20,350 ± 5,590
uniform Best solution found	2,355,900	2,951,000	3,365,400
gene-based Avg best solutions	2,134,480 ± 62,000	1,974,740 ± 32,600	1,940,060 ± 34,70(
gene-based # of objective-evaluations	4,420 ± 1,180	2,940 ± 2,170	300 ± 250
gene-based Best solution found	2,200,000	2,025,000	1,994,400

Table 9.10: Genetic algorithms performance on the multi-stage model with population size 50.

Crossover operator	Selection operator		
	Fitness Proportion	Stochastic Baker	Modified Tourname
1-point Avg best solutions	2,316,300 ± 45,200	2,910,090 ± 26,300	3,497,570 ± 42,00(
1-point # of objective-evaluations	11,750 ± 3,610	29,730 ± 260	21,840 ± 2,050
1-point Best solution found	2,366,200	2,946,900	3,544,200
2-point Avg best solutions	2,383,560 ± 50,400	2,799,740 ± 67,300	3,473,400 ± 42,00(
2-point # of objective-evaluations	16,490 ± 5,460	29,480 ± 650	19,750 ± 1,960
2-point Best solution found	2,465,400	2,928,700	3,531,200
uniform Avg best solutions	2,197,540 ± 27,300	2,708,300 ± 80,900	3,168,620 ± 37,80(
uniform # of objective-evaluations	4,920 ± 1,880	26,270 ± 4,300	18,040 ± 6,280
uniform Best solution found	2,239,400	2,858,500	3,229,400
gene-based Avg best solutions	2,125,020 ± 71,500	1,999,960 ± 39,900	1,953,720 ± 37,80(
gene-based # of objective-evaluations	5,740 ± 1,750	4,650 ± 2,650	560 ± 270
gene-based Best solution found	2,232,200	2,054,800	2,028,400

9.11 Experiment 8: Immune systems

Methods

The objective of this experiment is to test whether or not immune systems will improve the performance of GA or not? In this experiment, the optimal set of operators found for GA in

Table 9.11: Genetic algorithms performance on the multi-stage model with population size 60.

Crossover operator	Selection operator		
	Fitness Proportion	Stochastic Baker	Modified Tournament
1-point Avg best solutions	2,233,270 ± 50,400	2,859,640 ± 39,900	3,532,250 ± 30,500
1-point # of objective-evaluations	10,440 ± 3,640	29,740 ± 200	29,490 ± 1,210
1-point Best solution found	2,330,100	2,915,200	3,597,100
2-points Avg best solutions	2,315,250 ± 47,300	2,688,340 ± 72,500	3,502,820 ± 45,200
2-points # of objective-evaluations	15,370 ± 4,050	26,840 ± 4,300	24,830 ± 3,520
2-points Best solution found	2,368,700	2,790,100	3,566,300
uniform Avg best solutions	2,178,620 ± 35,700	2,732,480 ± 100,900	3,088,750 ± 44,100
uniform # of objective-evaluations	6,230 ± 3,340	27,100 ± 3,400	15,840 ± 4,690
uniform Best solution found	2,235,900	2,893,200	3,144,900
gene-based Avg best solutions	2,224,870 ± 78,800	2,001,010 ± 26,300	1,939,010 ± 28,400
gene-based # of objective-evaluations	10,080 ± 2,670	6,600 ± 3,090	680 ± 430
gene-based Best solution found	2,363,100	2,036,000	1,974,400

Table 9.12: Genetic algorithms performance on the multi-stage model with population size 70.

Crossover operator	Selection operator		
	Fitness Proportion	Stochastic Baker	Modified Tournament
1-point Avg best solutions	2,167,060±66,200	2,751,390±37,800	3,426,100±23,100
1-point # of objective-evaluations	7,700±4,490	28,900±370	28,940±270
1-point Best solution found	2,265,000	2,796,400	3,470,300
2-point Avg best solutions	2,261,650±52,500	2,632,630 ± 73,600	3,502,820 ± 25,200
2-point # of objective-evaluations	28,130 ± 1,710	28,130 ± 1,710	29,120 ± 150
2-point Best solution found	2,345,900	2,778,400	3,540,300
uniform Avg best solutions	2,163,910 ± 32,600	2,710,410 ± 65,200	3,045,660 ± 34,700
uniform # of objective-evaluations	6,170 ± 3,330	23,780 ± 4,660	15,600 ± 3,630
uniform Best solution found	2,224,400	2,854,700	3,128,200
gene-based Avg best solutions	2,336,270 ± 114,600	2,027,290 ± 32,600	1,971,590 ± 50,400
gene-based # of objective-evaluations	16,370 ± 4,970	7,740 ± 5,630	990 ± 720
gene-based Best solution found	2,528,000	2,067,500	2,071,100

Section 9.10 is used to set up the immune system experiment. The top 10 percent of the population is used as the antigens. The similarity measure is calculated by mapping each chromosome to the equivalent binary matrix representation (equivalent to the mating matrix M) and the hamming distance is calculated. The algorithm presented in Figure 6.8 is used while the adopted **compare_with_antigen_and_update_fitness**($P_{G=k}$) procedure is depicted in Figure 9.10. It is

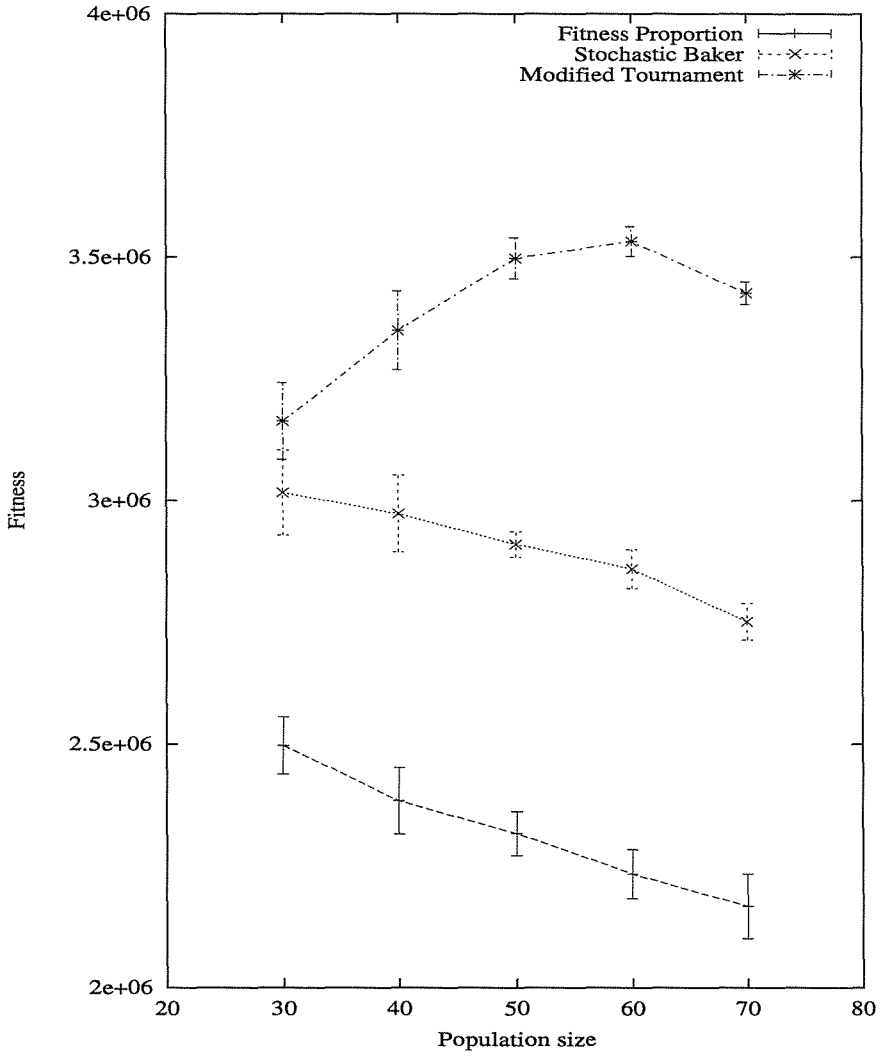

Figure 9.9: The performance of 1-point crossover using the three selection strategies over ten runs.

essential here to scale the similarity measure by dividing it by the chromosome length. The reason for this scaling is that the original objective values are small after scaling them. Therefore, if we directly add the hamming distance (which range from 0-1000; 5 stages $\times$ 200 dams) between the antigen and the antibody, stagnation will occur quickly because the hamming distance will dominate the original objective function.

Results and discussion

The immune algorithm is run for 30,000 objective-evaluations ten different times with different seed initialisations. The average of the best solutions found for the ten runs was 3,529,600 $\pm$

```
procedure compare_with_antigen_and_update_fitness(P_{G=k})
    Antigen = top 6 individuals in (P_{G=k})
    l = 0
    while l < 120
        randomly select y ∈ antigen
        Sim_opt = 0
        foreach , x' ∈ P_{G=k}
            if random(0,1) < 0.2 then
                Sim = similarity(y, x')
                if Sim > Sim_opt then Sim_opt = Sim, x = x'
        add similarity(y,x)/1000 to the fitness of x ∈ P_{G=k}
        l = l + 1
end procedure
```

Figure 9.10: The antigen-antibody comparison algorithm

45,200. This solution was found after 28,740 $\pm$ 1,640 objective-evaluations on the average. The best solution among the ten runs was 3,568,200. Therefore, the immune system did not improve the performance of GA. In Table 9.13, the solutions found in each of the ten runs is given. We may notice that the second and ninth runs were the worst which explains the bad performance of Immune relative to GA.

Table 9.13: The Immune algorithm's performance on the multi-stage model

Run	1	2	3	4	5
Solution	3,552,500	3,452,900	3,563,700	3,548,400	3,537,400
Run	6	7	8	9	10
Solution	3,550,500	3,543,600	3,540,900	3,437,600	3,568,200

9.12 Experiment 9: Evolving colonies of ants (a new algorithm)

Methods

In this experiment the optimal set of operators found for GA in Section 9.10 is used in conjunction with the ACO to set up the hybrid algorithm. The goal here is, instead of improving each ant independently, GA is used to evolve the ants instead. The algorithm is depicted in Figure 9.11. In the first generation, five ants are generated using the pheromone table. The colony of ants evolves (by means of crossover) for 96 objective-evaluations, then all ants die but the fittest ant, which is preserved in the colony. The reason for choosing 96 objective-evaluations is that only 4 ants are generated, and consequently evaluated, in subsequent iterations since the fittest ant is always kept. Therefore, in each cycle, 100 objective evaluations are undertaken. Although the best performance for the ant algorithm occurred with 1 ant, we use five ants here to have a population.

Results and discussion

The algorithm is run for up to 300 cycles with a condition that the last improvement in the best solution found does not take place for more than the last 30 cycles, where in each cycle, 100 objective evaluations are undertaken as previously mentioned in order to preserve the maximum of 30,000 objective evaluations. It is found that the algorithm resulted in a better solution than GA and ACO in isolation. The results are statistically different at 99.9% confidence level using the correlated paired t-test. The t values were 93.44 and 4.99 for ACO and GA respectively. The average best solutions found for the ten runs was 3,579,540 $\pm$ 25,200. This solution was found after 29,700 $\pm$ 160 objective-evaluations on the average. The best solution among the ten runs was 3,615,100. Therefore, this method overcomes the scalability problem in ACO and improves the performance of GA.

```
procedure ACO_heuristic()
    initialise pheromone_table
    while (termination_criterion_not_satisfied)
        for ant k = 1 to 5 do
            if objective − evaluation > 1 and k is not the fittest ant then
                initialise_ant();
                M ← update_ant_memory();
                Ω ← a set of problem's constraints
                while (current_state ≠ target_state)
                    A = read_local_ant-routing_table();
                    P = compute_transition_probabilities(A,M,Ω);
                    next_state = apply_ant_decision_policy(P, Ω);
                    move_to_next_state(next_state);
                    M ← update_internal_state();
        for i = 1 to 96 do
            crossover two ants at random
            if the child is better than the worst ant in the population
                replace the child with the worst ant in the population
        foreach ant in the population
            foreach visited state do
                deposit_pheromone_on_the_visited_arc();
                update_ant_routing_table();
        Update_the_pheromone_table();
        kill all ants except the fittest
end procedure
```

Figure 9.11: A heuristic for evolving colonies of ants

9.13 Overall discussion

In Table 9.14, the best results obtained in each experiment is summarised together with the t-value obtained from comparing the experiment with the best strategy (Markov Chain Tabu Search) using the correlated paired t-test[1]. Also in Figure 9.12, the performance of the best combination found with each heuristic is plotted. It is found that the results in all experiments are statistically different from the MCTS strategy at confidence level 0.999. Therefore, it is a simple matter to conclude that MCTS was the best strategy for the mate-selection problem presented in this thesis.

[1]The correlated version of the paired t-test is used here since in the ten runs, the same seeds were used. Therefore, the results of all experiments are dependent and the correlated test should be used not to over or under-estimate the t-value. A complete description of the test is provided in Runyon et al. (1996).

One should be careful in interpreting the results of these experiments. As we used a fixed number of objective evaluation, the results may change if we increase the number of objective evaluations. However, we cannot wait until each algorithm converges as this may take forever. Therefore, using a fixed number of objective evaluations is a fair thing to do. Also, since the number of objective evaluations is fixed, the CPU time is almost the same among the different algorithms. The reason is that the overhead of each algorithm is negligible compared to the time of evaluating a solution.

Table 9.14: A summary of the best combination found in each experiment and its corresponding t-value relative to the MCTS algorithm

Experiment	Avg best solutions	# of objective-evaluations	Best solution found	t-value
Markov Chain TS	3,805,500 ± 13,700	29,910 ± 110	3,824,600	
Evolving colonies of ants	3,579,540 ± 25,200	29,700 ± 160	3,615,100	23.48
GA	3,532,250 ± 30,500	29,490 ± 1,210	3,597,100	23.43
Immune	3,529,600 ± 45,200	28,740 ± 1,640	3,568,200	18.18
Hill climber	3,510,180 ± 15,800	29,600 ± 350	3,533,000	46.87
Sequential GA	3,429,260 ± 30,500	N/A	3,483,700	47.97
SA	2,407,730 ± 34,700	2,370 ± 950	2,493,000	94.29
Ant Colony	2,345,670 ± 32,300	3,200 ± 2,900	2,414,900	189.44
Random	2,013,620 ± 23,100	2,940 ± 1,710	2,058,400	199.10

The results of this chapter are very interesting. Conventional ACO suffered from a scalability problem and performed very badly relative to SA. However, when merged with GA, the hybrid algorithm performed the best after MCTS. This finding required some interpretations. We know from Chapter 6 that SA uses Markov chains and if it is given enough time, it will converge.

ACO also depends on a Markov chain. To observe this, let us momentarily ignore the local search procedure used to improve the ants performance. Moreover, let us forget the ants and just concentrate our attention on the normalised pheromone matrix that we may envisage as the ants' vision of the probability distribution of the transitions an ant needs to take to find the best solution found in the world. The ants are generated based on this probability matrix (prior distribution) that is then updated based on what the ants have found (posterior distribution). Let us sum all the updates in a single objective-evaluation in one matrix and let us normalise this matrix. The ants algorithm can be now seen in terms of these two matrices: the

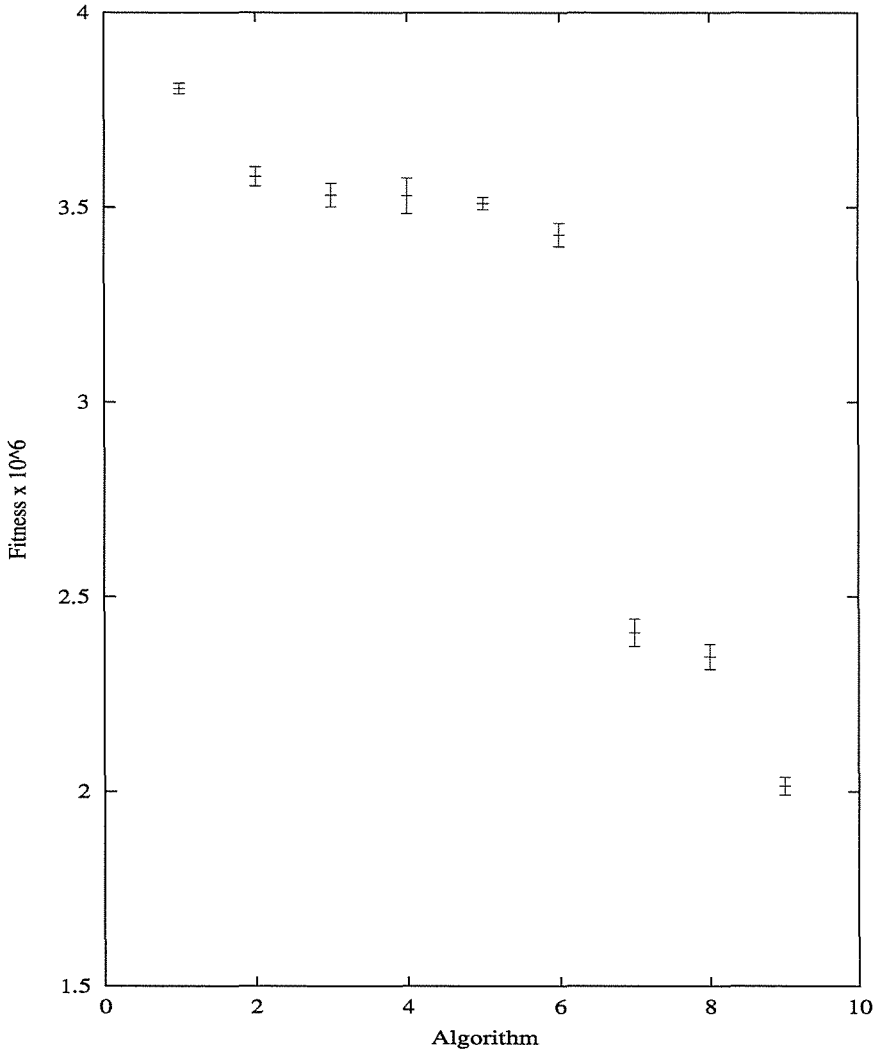

Figure 9.12: The performance of the best results obtained by different algorithms.
The x-axis represents the heuristic; 1-MCTS, 2-Evolving colonies of ants, 3-GA, 4-Immune, 5-Hill climbing, 6-Sequential GA, 7-SA, 8-ACO, 9-Random. The y-axis is the average fitness of ten runs.

normalised pheromone matrix and the normalised update matrix. In each objective-evaluation, the normalised pheromone matrix is updated based on the normalised update matrix. The new pheromone matrix depends only on the previous one; therefore a Markov characteristic is inherent to ACO.

MCTS can also be seen as a series of Markov chains, where the probabilistic tabu list is updated in each objective-evaluation and the new one depends only on the previous one. The real difference between ACO, TS, and MCTS is that ACO uses positive knowledge only with a positive search strategy (*ie.* keep rewarding good solutions and bias the search towards these good areas), TS uses negative knowledge only with a positive search strategy (*ie.* prohibiting previously visited states and bias the search to previously un-visited and potentially good states), but MCTS uses both types of knowledge (positive and negative) with a positive search strategy (*ie.* rewarding good solutions, penalising bad solutions, and biasing the search towards potentially good areas). SA is somewhat different since it does not use any of these knowledge but instead uses a mixture of positive and negative search strategies with a certain probability. To illustrate this point, in the beginning of the search, SA emphasises a negative search strategy since it accepts bad steps most of the time while the temperature is high. In the end of the search, the situation is reversed. However, there is no guarantee that this is always good. Perhaps a negative or positive knowledge is more important during the search in some problems. This may provide an interpretation of the better performance achieved when using MCTS.

I have illustrated in the previous discussion that SA, ACO, and MCTS have a Markovian characteristic. Therefore, when the search space is huge, as in our case, any of these algorithms is expected to need so much time to reach equilibrium; a problem that does not exist with GAs. However, MCTS performed the best due to the search intensification through a continuous reward for the best solution found and a continuous penality for bad solutions.

GAs easily outperformed SA and ACO since it survived the condition of an improvement every 3,000 objective evaluations. SA and ACO did not survive this condition because they were behaving like random search to explore the search space. The temperature of SA did not have time to cool and the pheromone matrix of ACO did not have time to reach a steady state. In GA,

the selection pressure resulted from the modified tournament strategy proved to have a positive effect in our problem. Also, the 1-point crossover operator managed successfully to sustain good schemas while the repair operator adds some mutations from time to time when feasibility is broken by recombination.

Immune systems did not improve the performance of GAs. With the pressure introduced by the similarity measure, the schemas inherited in the best solutions in each stage are rewarded in the rest of the population. This type of pressure may have been beneficial if it is given enough time. However, in our case, it did not improve the performance of GAs. Surprisingly enough, the results obtained from the immune algorithm were statistically different from the MCTS algorithm with a t-value lower than that obtained for GAs. After investigating this case, it was found that in one of the ten runs, the behaviour of the immune algorithm dropped dramatically while the behaviour of GAs using the same seed was very good [2]. However, in seven out of the ten runs, the immune algorithm was better than its corresponding GAs.

The ACO+GA algorithm presented another successful step to improve the performance of GA and to overcome the scalability and slow convergence problems of ACO. MCTS gave the best results overall and achieved significantly better solutions than all other algorithms. It is therefore chosen as our preferred strategy for solving the version of the multi-stage mate-selection problem presented in this thesis.

One last important issue needs still to be discussed here; that is, the practicality of the model solved in this chapter. This issue will be argued using questions and answers.

Q: Does it make sense that certain algorithms are better suited for solving the mate-selection problem than others?

A: This is a very important question concerned with the problem's features which make an algorithm more suitable for the problem than another. The mate-selection problem is similar

[2]This was the seed where the best solution of GAs over the ten runs was obtained. Also, it was the seed corresponding to the worst immune algorithm's performance.

to many combinatorial optimisation problems. Therefore, it is difficult to say when a heuristic will work and when it will not objectively. However, I might give here a guideline to assist the practitioners. The problem in hand is a large scale problem, therefore the search space is huge. Even with a greedy local search algorithm, it will take very long time to reach a local optimal solution. In practice we don't have such time given that we will get a weak local optimal solution. Obviously, the ideal situation is to get the global optimal solution but the practical one is to get a better local optimal solution. On the one hand, population based heuristics, such as genetic algorithms, depend on the diversity in the population to better sample the search space. But when a huge search space exists, a fair sample of the search space is very costly and the convergence is slow. For a non-population based heuristics, such as simulated annealing, ant colony, and tabu search, the huge search space causes a scalability problem. SA and ACO will need a tremendous time to reach equilibrium. The conventional TS approach will not work because of the large size of the neighbourhood. To see this last point, assume our solution's representation is of length 1000 and we define the neighbourhood by a two cells' change; therefore the neighbourhood size is bounded with $O(1000^2)$. Actually in this case it is around 10^5. In this huge neighbourhood, what is the probability of cycling? It is almost zero. Therefore, we need huge memory to handle this problem. The obvious question now is why did the MCTS algorithm work? Because in MCTS, the neighbourhood is centred on the best solution found so far and is defined by the overall search space; that is, any point in the search space is reachable from the best solution found so far. However, not every point is reachable with the same probability. After the algorithm performs a number of iterations, the probability transition matrix restricts the search space. To forbid quick stagnation, some random values are added to the probability matrix so that the matrix itself does not trap in a local optimum. The update of the matrix is undertaken by a double re-inforcement approach (penalising bad solutions and rewarding good ones.). This approach of global intensification of the search seems to be very benefecial in the mate-selection problem. Therefore, I would suggest a carefully designed re-inforcement approach, such as MCTS, for the mate-selection problem.

Q: How can the model take into account the probability of conception failure?

A: Let us assume that the farmer requires ten matings and the probability of conception failure

is 10%, the farmer may ask the system for eleven matings instead; therefore, overcoming the risk of conception failure. It is important here to recognise that this method, although very simple, does provide a practical approach to handle the problem of conception failure. The reason is that it is not clear which cow will suffer from this problem (unless we have a trait for cow's conception). Therefore, we may seek the best eleven matings, assuming that one will fail.

Q: How can the model take into account the gender of the progeny?

A: How can we tell in advance if the result of a mating will be a male or a female? This is a difficult question and the same trick, of the previous question, will be used. Assume that we require fifty daughter. We may ask for the best one hundred matings instead, therefore with a probability 0.5, the expected number of daughters will be 50 as required. Note that in reality, the farmer does not know in advance if a mating will take place or not, if the outcome of a mating is a male or a female, or if the progeny will live or die. Therefore, over-estimating the number of required matings is a wise strategy, as long as it is reasonable; otherwise the farmer will do unnecessarily matings which represent cost on the farm. This point is outside the scope of the thesis; however, an economic model for this type of decisions can be an interesting piece of research for future work.

Q: Is there a difference between optimising two stages or five stages?

A: This question arises from discussions regarding the reason for more than two-stage optimisation. The answer is that by minimising the problem for five stages, we require enough variance in the first generation's assignment so that inbreeding is minimum over the 5 generations. However, we can get a similar effect if we increase the weight of inbreeding in the two-stage optimisation. Actually, we do not need to optimise initially for two stages and one stage would be sufficient if we know the right combination of weights. Notwithstanding, we cannot know the right combination of weights without building sophisticated economic models for each herd independently. Therefore, adding more generations will add implicitly more weights on short and long term inbreeding.

To further illustrate our point, we need an experiment. The best set of parameters obtained by MCTS (using the seed corresponding to the best solution found for MCTS) was used to optimise

the same problem we presented in this chapter for 2, and 5 stages. The matings of the first stage in each of the two experiments are reported here in order to observe the impact of multi-stage optimisation on the first stage. We should expect that the more stages we optimise, the more the population is penalised for inbreeding. Therefore, we should expect lower inbreeding (higher variance) and lower expected breeding values (as a result of penalising the matings for long term inbreeding). The results of this experiment are presented in Table 9.15. The numbers in this figure are approximated for three significant numbers.

Table 9.15: The effect of the number of stages on the optimisation process.

Objective	Two Stages	Five Stages
O1: Production	632000	631000
O2: Inbreeding	-17	-16
O3: Breeding Values	69300	69200
O4: Coancestry	-5870	-5860

As can be seen from the table, the production and breeding values for the two-stage model are higher than that for the five-stage model, and inbreeding is also higher. However, we have to say that to test if this result is statistically significant or not, one needs to carry out a number of runs. In any case, whether we optimise for two or more generations, the purpose of this chapter is to discuss the problem from optimisation point of view. As will be suggested in the last chapter of the thesis, an interesting piece of research for future work would be to analyse the results of this thesis within an economic model to generate appropriate weights, for the objective function, that will influence the results of the optimisation model. Such a model is outside the scope of the thesis and is proposed for future work.

9.14 Conclusion

This chapter is concerned with the third sub-objective of the thesis; solving the proposed version of the multi-stage mate-selection problem presented in this thesis. Nine different heuristic techniques, two of which (evolving colonies of ants and Markov chain tabu search) were newly developed in this thesis, are used to solve the problem. The MCTS is significantly better than the rest and resulted in the best overall performance.

Chapter 10

Generation of Mate-selection Index

The main objective of this chapter is to generate a mate-selection index. The mate-selection index is introduced in Section 10.1 followed by a mathematical proof for the existence of this index in Section 10.2. In Sections 10.3 and 10.4, two methods are envisaged for generating this index using an SA+GA hybrid and DE+GA hybrid respectively. The chapter is concluded with Section 10.5.

10.1 Mate-selection Index (MSI)

An index for mate-selection is suggested by Kinghorn et.al. (1999). In their paper, the index ranks the animals according to their potential as mating animals. They showed that such an index is very beneficial and it is different from the conventional selection index, because the latter does not account for issues like inbreeding, coancestry, and mate-selection, whereas the MSI does. This chapter is about the generation of MSI. However, MSI is defined here as a vector of weights rather than ranks as in Kinghorn et.al. (1999). Therefore, the problem discussed in the current chapter is to find a vector of weights (a single weight for each animal) such that if the mate-selection problem is optimised for each stage independently using the MSI vector (referred to by $R(t)$ for stage t or simply R for all stages) to form a linear objective function $(\sum_{t=0}^{T} R(t) \times [X(t)Y(t)])$ for the breeding program, the result will be the optimal solution of the multi-stage problem using the aggregated objective defined in Section 9.3.4. Therefore, the weights in the MSI hides the contribution of each animal in terms of the four objectives defined in the previous chapter. This problem is more complex than the multi-stage problem presented

in the previous chapter. To find the MSI, we have two search spaces; the first is to search for the MSI vector, and the second is the multi-stage problem presented in the previous chapter using the MSI vector as the objective function coefficients. To explain the concept of this problem, let us recall that the sequential GA method in the previous chapter failed to give the best solution for the multi-stage problem because of the interaction between the objectives over stages. Therefore, what we are looking for is a linear objective function which if used to optimise each stage independently, the result would be the optimal solution of the multi-stage problem using the four objective functions defined in Section 9.3.4. The coefficients of the animals in this linear function is the MSI vector. Based on this discussion, a heuristic search may proceed as follows:

1. find an MSI $R(t)$ for each stage t,
2. optimise the objective function for each stage independently using $\sum_{t=0}^{T} R(t) \times [X(t)Y(t)]$,
3. evaluate the resultant solution using the aggregated nonlinear function from the previous chapter, Equation 9.1, then
4. keep adjusting $R(t)$ for all stages t such that the resultant solution using the aggregated nonlinear function is as maximum as possible.

This approach will be called *dynamic adjustment of the objective function.* It is easy to see that the complexity of the problem increased because the continuous search space of the linear objective functions (MSIs) added complexity to the original search space of animal allocations. However, four questions remain to be answered before attempting to solve this problem:

1. Does the MSI as defined here exist?
2. If it exists, does it guarantee the optimality of the mate-selection problem?
3. If it does, how can we generate such an index?
4. Is it unique?

The answers to these four questions are the foci of this chapter. In the next section, It will be proven mathematically that this index exists and does guarantee the optimality of the problem. Also, it will be shown that this index is not unique. Two attempts for finding this index are carried out later in the chapter.

10.2 Dynamic adjustment of the objective function (a new algorithm)

Let us define the multi-stage binary optimisation problem P1 as follows:

$$Minimise \quad \sum_{t=0}^{T} f(x(t)) \tag{10.1}$$

Subject to

$$G(x(t)) \leq 0 \quad t = 0, \ldots, T \tag{10.2}$$

$$x_i(t) \in \{0, 1\}, \quad i = 0, \ldots, n, \; t = 0, \ldots, T \tag{10.3}$$

Now, define the single-stage binary optimisation problem P2(t) for stage t in P1 as follows:

$$Minimise \quad f(x(t)) \tag{10.4}$$

Subject to

$$G(x(t)) \leq 0 \tag{10.5}$$

$$x_i(t) \in \{0, 1\}, \quad i = 0, \ldots, n \tag{10.6}$$

Lastly, define the relaxed single-stage optimisation problem P3(t) which corresponds to P2(t) as follows:

$$Minimise \quad f(x(t)) \tag{10.7}$$

Subject to

$$G(x(t)) \leq 0 \tag{10.8}$$

$$0 \leq x_i(t) \leq 1, \quad i = 0, \ldots, n \tag{10.9}$$

Lemma 1:

If an optimal feasible solution exists for P1, then $\exists$ a transformation function α_t for $f(x(t)) \ni$ if $x^*(t)$ is the optimal solution of $Minimise \quad \alpha_t(f(x(t)))$, s.t. $G(x(t)) \leq 0$; $t = 0, \ldots, T$ and $x_i(t) \in \{0, 1\}, i = 1, \ldots, n$, then $x^*(t)$ is the optimal solution of P1.

Proof

The proof of this lemma is very straight forward. The real problem with P1 is there's no guarantee that by optimising every stage independently, the optimal solution for each stage will be an optimal solution for P1. That is, if $x^+(t), t = 1 \ldots T$ is the optimal solution of P2(t), $t = 1 \ldots T$, then there is no guarantee that $x^+(t), t = 1 \ldots T$ is the optimal solution of P1, because of the interaction among the stages. But if the optimal solution for P1, $x^*(t)$, exists, then $x^*(t)$ must be a feasible solution of P2(t). Since any feasible solution is also optimal for some objective functions, this implies that there must be an objective function $f^*(x(t))$ such that $x^*(t)$ is the optimal solution of *Minimise* $f^*(x(t))$, s.t. $G(x(t)) \leq 0; \quad t = 0, \ldots, T$ and $x(t) \in \{0, 1\}$ [1]. But this implies that $\exists$ a transformation function α_t for $f(x(t)) \ni \alpha_t(f(x(t))) = f^*(x(t))$. $\diamondsuit$

Lemma 2:

> $\exists f^*$, a linear function, $\ni$ if $x^*(t)$ is the optimal solution of P3(t) under f^*, then $x^*(t)$ is the optimal solution of P1.

Proof

In Lemma 1, it was shown that $\exists$ an objective for each P2(t) which if used to optimise each P2(t) independently, the result is the optimal solution of P1. In the current lemma, it will be shown that $\exists$ a linear version of this objective but for P3(t). But this is true since P3(t) is the relaxed version of P2(t). To make this clear, we have the constraint $0 \leq x(t) \leq 1$ in P3(t) which will result in a hypercube. But we know from the theory of linear programming that the optimal solution is always on an extreme point of the polyhedra of the feasible solutions' set. Since P2(t) is binary, then all feasible solutions for the problem are located on the extreme point of the polyhedra, the feasible solutions set for P3(t). This entails that for any feasible solution, $x^*(t)$, for P2(t), $\exists$ a linear objective $f^* \ni$ by optimising P3(t) using f^*, the optimal solution is $x^*(t)$. $\diamondsuit$

[1] An obvious objective is a circle centred on $x^*(t)$ with a zero radius

The MSI

The previous two lemmas proved that there is always a linear function, representing the mate-selection index, that if used to optimise each stage independently, the optimal solution of each stage is also optimal for the overall mate-selection problem. However, this linear function is not unique since there are many linear functions which can result in the optimal solution because the extreme point of the hypercube is insensitive to some degree of change in the linear objective function. Therefore, MSI exists, guarantees the optimality of the mate-selection problem, and is not unique. Based on these lemmas, the dynamic adjustment method starts with a randomly generated MSI (or population of MSIs for the population based heuristic) vector and dynamically adjust (by rotation) this vector until the optimal solution is found. The following two sections present two attempts to find the MSI using a hybrid of SA and GA and a hybrid of DE and GA. Both SA and DE are chosen because of their suitability for continuous optimisation.

10.3 Hybrid SA + GA

Methods

A hybrid GA and homogeneous SA algorithm is employed in this strategy. The SA part is rotating an initial randomly generated vector (R) linear objective while the GA component is undertaking a short run-cycle to optimise each stage independently using sequential GA (function **GA1** as described in Section 9.5 with the linear objective generated by SA in Figure 10.1). The result of the sequential GA is then evaluated using the aggregated function from the previous chapter (the same linear combination of the four objective functions presented in Section 9.3.4 (Equation 9.1) is used, with $\alpha = 1$, $\beta = 1$, $\gamma = -1$, and $\delta = -1$).

The hybrid algorithm is shown in Figure 10.1. The algorithm starts with the initial temperature T as an input from the user. The chain length L is initialised to 1000 and the number of coolings C to 100. This setup together with a decrement in the chain length of 0.968 guarantees a maximum number of objective evaluations of 30,000 (refer to Section 9.7). The temperature is decremented by a constant equal to the initial temperature divided by the total number of coolings. At the start, a linear function R_0 is initialised randomly from a uniform distribution

between 0-1. Simulated annealing is then used to rotate R_i using the function **rotate** which randomly changes 10% of the values in R_i by adding to each of these values a uniformly distributed random number between 0-0.1. Each time the linear function R_i is generated, sequential GA, function **GA1**, is used to optimise the problem using the linear function R_i. The sequential GA consists of a population of 20 individuals and run for 50 GA-generations using 1-point crossover and the modified tournament strategy. The number of GA-generations is chosen based on the results shown in Figure 8.4 where in the first 50 GA-generations, GA improved the solution very fast. Also, we reduced the population size to increase the pressure so that we get a fast estimate. The number of objective evaluations carried out by the function $GA1$ are not being accounted for in the 30,000 objective-evaluations condition. The reason for that is $GA1$ uses a linear function which can be evaluated in a negligible time compared to the evaluation time needed by the aggregated function where inbreeding and coancestry are calculated. We may note that the functions $f_{new}(x)$, $f_{current}(x)$, and $f_{opt}(x)$ evaluate a solution using the original aggregated function (Equation 9.1).

To gain an insight about an appropriate value for the initial temperature, 10 runs of length 200 objective evaluations were made. It was found that 99% of the solutions can be accepted with average temperature of 70. Consequently, three initial temperature levels (70, 40, and 1) are experimented with. Therefore, a total of 3 experiments is carried out, with each experiment runs ten different times with different seeds. A maximum of 30,000 objective evaluations were set on each run with a stop occurring either when this maximum is reached or when 3000 objective evaluations elapse without an improvement in the best solution found.

Results and discussion

The results of this experiment are shown in Table 10.1. It can be seen from the table that the algorithm is similar to random search, since it was incapable of improving the results obtained from random search in the previous chapter. The reason behind this is that the complexity of the search problem is increased. The additional search for the MSI added a burden to the original search for the best solution found. The results are not statistically significant. The best value obtained in this experiment is associated with temperature level 40 where the average of

function *SA+GA*
Input: T
$C = 100$, $L = 1000$, $i = 0$
Generate R_0 *at random*
initialise best solution found R_{opt} *to be* R_0
initialise current solution $R_{current}$ *to be* R_0
$x_{current} \leftarrow \mathbf{GA1}(R_0)$
$x_{opt} \leftarrow x_{current}$
$f(x_{opt}) \leftarrow f(x_{current})$
temperature_step $= T/C$
for $k = 0$ *to* C
for $j = 0$ *to* L
$i = i + 1$
$R_i \leftarrow \mathbf{rotate}(R_{current})$
$x_{new} \leftarrow \mathbf{GA1}(R_i)$
$\Delta(f) = f(x_{new}) - f(x_{current})$
if $f(x_{new}) > f(x_{opt})$ **then** , $R_{opt} = R_i, x_{opt} = x_{new}$, $f(x_{opt}) = f(x_{new})$
if $f(x_{new}) > f(x_{current})$ **then** , $R_{current} = R_i, x_{current} = x_{new}$, $f(x_{current}) = f(x_{new})$
else if $exp(\Delta(f)/T) >$ *random (0,1)* **then** $R_{current} = R_i, x_{current} = x_{new}$, $f(x_{current}) = f(x_{new})$
if *last update of* $f_{opt} > 3000$ **exit for**
$T = T -$ *temperature_step*
$L = L * 0.968$
if *last update of* $f_{opt} > 3000$ **exit for**
return *the best MSI found* R_{opt}
end function

Figure 10.1: A Hybrid GA+SA algorithm for generating of mate-selection index.

the best solutions in the ten runs is 1948470 ± 37800 and is found on the average at iteration 2230 ± 1480. The best solution found during the experiment is 2029600. The SA algorithm could not survive the condition of improving the best solution found within each 3,000 objective evaluations and therefore terminated early.

Table 10.1: Results of GA/SA Hybrid for MSI. Columns represent the three different temperature levels.

Criteria	Temperature		
	70	40	1
average fitness	1,939,010 ± 28,400	1,948,470 ± 37,800	1,937,960 ± 22,100
average # iterations	1,840 ± 1,910.0	2,230 ± 1,480.0	1,710 ± 1,200.0
Best solution	2,002,000	2,029,600	1,966,400

10.4 Hybrid DE + GA

Methods

A hybrid GA and DE algorithm is employed in this strategy and shown in Figure 10.2. The algorithm starts with two inputs from the user, the crossover probability CR and the step size F. The GA consists of a population of 20 individuals and run for 50 GA-generations using 1-point crossover and modified tournament strategy. The initial population of MSIs (R) in DE is initialised randomly from a uniform distribution between 0-1. The DE part is rotating the initial population of MSIs (R) using crossover, while the GA component is undertaking a short run-cycle to optimise each stage independently. Differential evolution is described in Section 6.5.

Four crossover probabilities of 1.0, 0.8, 0.4, and 0.1 and three step sizes of 0.8, 0.4, and 0.1 were used to conduct 12 experiments, with each experiment runs ten different times with different seeds. A maximum of 30,000 objective evaluations were set on each run with a stop occurring either when this maximum is reached or when 3000 objective evaluations elapse without an improvement in the best solution found.

Results and discussion

The results of this experiment are shown in Table 10.2. Once more, it can be seen from the table that the algorithm is similar to random search although it was capable to improve the results obtained from SA+GA in the previous section. The results are not statistically significant. The best value obtained in this experiment is associated with crossover probability 0.8 and step size 0.8. The average of the best solutions in the ten runs is 1962130 $\pm$ 37800 and is found on the average at iteration 3910 $\pm$ 3310. The best solution found during the experiment is 2030900. The DE algorithm could not survive the condition of improving the best solution found within each 3,000 objective evaluations and therefore terminated early.

function *DE+GA*

Input: *CR and* $F \in (0,1)$

let G denote a DE-Generation, P a population of size M, and $R^j_{G=k}$ *the jth individual of dimension N in population P in stage k, and CR denotes the crossover probability*

initialise $P_{G=0} = \{R^1_{G=0}, \ldots, R^M_{G=0}\}$ *as*

foreach *individual* $R^j_{G=0} \in P_{G=0}$

foreach $i \in N$

$R^j_{i,G=0} = random(0,1), i = 1, \ldots, N$

$x_{new} \leftarrow$ **GA1**$(R^j_{G=0})$

let the fitness value, $F(R^j_{G=0})$*, of* $R^j_{G=0}$ *be* $f(x_{new})$

k=1;

while *the stopping criterion is not satisfied* **do**

forall $j \leq M$

randomly select $r_1, r_2, r_3 \in (1, \ldots, M), j \neq r_1 \neq r_2 \neq r_3$

randomly select $i_{rand} \in (1, \ldots, N)$

$$\forall i \leq N, R'_i = \begin{cases} R^{r_3}_{i,G=k-1} + F \times (R^{r_1}_{i,G=k-1} - R^{r_2}_{i,G=k-1}) & if \quad (random[0,1) < CR \wedge i = i_{rand}) \\ R^j_{i,G=k-1} & otherwise \end{cases}$$

$x_{new} \leftarrow$ **GA1**(R')

let the objective value, $F(R')$*, of* R' *be* $f(x_{new})$

$$R^j_{G=k} = \left\{ \begin{array}{ll} R' & if\ F(R') \leq F(R^j_{G=k-1}) \\ R^j_{G=k-1} & otherwise \end{array} \right\}$$

$k = k + 1$

return *the best encountered MSI* $R \in P_{G=k}$.

end function

Figure 10.2: A Hybrid GA + DE algorithm for generating of mate-selection index.

10.5 Conclusion

This chapter shows that the MSI exists and that it guarantees the optimality of the original mate-selection problem. However, the experiments show that searching for this index increased the complexity of the mate-selection problem and as a result, the best solutions found here were inferior to those obtained directly in the previous chapter. More precisely, it is inferior to the random search procedure presented in the first experiment of the previous chapter. A number of alternatives maybe investigated to improve the results of this chapter. For example, using linear programming instead of the sequential-GA module. Also, trying gradient-based optimisation techniques might be a worthwhile attempt. These suggestions are left for future work.

This chapter concludes the third sub-objective of the thesis; that is, formulating and solving the mate-selection problem. This sub-objective is achieved by formulating a general multi-stage mate-selection model in Chapter 7 which is then customised and solved to a single-stage model in

Table 10.2: Results of GA+DE Hybrid for MSI.

Criteria	Step size		
	0.1	0.4	0.8
crossover probability = 0.1			
average fitness	1,946,360 ± 22,100	1,939,010 ± 17,900	1,952,670 ± 17,900
average # iterations	2,820 ± 2,220	1,120 ± 1,270	3,830 ± 1,280
Best solution	1,981,400	1,982,400	1,981,000
crossover probability = 0.4			
average fitness	1,949,520 ± 29,400	1,940,060 ± 15,800	1,944,260 ± 20,000
average # iterations	2,320 ± 1,580	2,920 ± 2,340	690 ± 850
Best solution	2,010,400	1,968,000	1,982,100
crossover probability = 0.8			
average fitness	1,941,110 ± 12,600	1,935,850 ± 22,100	1,962,130 ± 37,800
average # iterations	1,680 ± 1,370	2,180 ± 2,150	3,910 ± 3,310
Best solution	1,969,900	1,976,100	2,030,900
crossover probability = 1.0			
average fitness	1,945,310 ± 18,900	1,943,210 ± 17,900	1,947,410 ± 34,700
average # iterations	1,700 ± 1,580	2,080 ± 1,800	2,390 ± 2,320
Best solution	1,983,900	1,974,200	2,024,900

Chapter 8 and to a multi-stage model for artificial insemination programs in Chapter 9. Lastly, the concept of mate-selection index is the context of this chapter.

Chapter 11

Conclusion and Future Work

11.1 Summary

This thesis has investigated the problem-solving techniques for the efficient design of dairy cattle breeding programs. To achieve this, a generic information system framework (KDD-IDSS) was established, through the integration of knowledge discovery from databases with intelligent decision support systems, to identify the crucial component of a breeding program's information system. To this end, three sub-objectives were identified:

1. designing a generic kernel (*ie.* an interface language between the system's components) for the KDD-IDSS,

2. discovering patterns in the dairy database using KDD, and

3. formulating and solving the version of the mate-selection problem presented in this thesis.

The first sub-objective was achieved by designing a meta-language, using the constraint logic programming paradigm, to integrate operations research and artificial intelligence modules within a KDD-IDSS. KDD enables the IDSS paradigm to update its knowledge and models dynamically, and therefore, provide up-to-date knowledge and models to improve the decision making process. An example obtained from the dairy industry of the language's implementation was discussed.

The second sub-objective was achieved by experiments involving point and interval function estimation. Point function estimation methods provide a value prediction for the expected progeny

milk production. Interval function estimation methods provide an explanation capability for the system regarding the prediction it makes. Artificial neural networks and linear regression were used for point estimation and rule extraction from artificial neural networks (RULEX) and the decision tree classifier (C5) were used for interval estimation. The prediction accuracy of the artificial neural network method was similar to that of the linear regression model. Since the linear regression model is simple and as accurate as the artificial neural network model on the used dairy database, it was chosen as the best model. For the interval estimation experiments, C5 had less rules than RULEX on the discrete inputs; therefore suggesting that C5 is more suitable for this estimation task. These experiments motivated the development of a new algorithm, C-Net, for generating multivariate decision trees. This algorithm achieved a performance intermediate between artificial neural networks and univariate decision trees. It was intermediate because it was better than C5 in terms of generalisation and sometimes generalised better than the neural network itself. Also, it was more expressive than the neural network but less expressive than the corresponding univariate decision tree. In this algorithm, we also introduced for the first time the concept of recurrent decision trees, where conventional decision trees were extended with some recurrent features.

The third sub-objective of the thesis was achieved by developing a generic formulation of a mate-selection problem called the evolutionary allocation problem (EAP). The EAP was found to be very complex. Table 11.1 summarises the complexity of the mathematical models presented in this thesis, as well as the complexity of a benchmark problem (traveling salesman problem). The representation for the heuristic techniques removed redundancy from the optimisation model without excluding any optimal solution; therefore, the optimisation model's search space was preserved within the heuristic techniques' representation. One can also see in the table that the search space of the multi-stage problem is similar to a traveling salesman problem with 500 cities. However, there are a lot of redundancy in the traveling salesman's search space using the representation that obtained the complexities presented in the table. In the multi-stage customised version of the EAP problem, the representation is very compact and therefore represent larger space. In summary, the multi-stage mate-selection problem is non-trivial and hides many complexity issues.

	Mathematical Programming	Heuristic
General EAP	10^{70335}	NA
Single-Stage	10^{660}	10^{208}
Multi-Stage	10^{66828}	10^{1000}
Sym. TSP (200 cities)	10^{374}	10^{374}
Sym. TSP (500 cities)	10^{1134}	10^{1134}

Table 11.1: The complexity of different mate-selection models.

To solve the multi-stage mate-selection problem, we compared nine techniques, where two of them were newly developed in this thesis. My two proposed techniques, called evolving colonies of ants and Markov chain tabu search, outperformed the other techniques. MCTS achieved results which were statistically significantly better than all the others. The mate-selection index was also investigated (Chapter 10) and the theoretical proofs for its existence and non-uniqueness were provided.

From a research perspective, the thesis represents a multi-disciplinary research project. To make the thesis readable by people from different backgrounds came at the cost of having a long, but still compact, document. In what follows, the contributions of the thesis are visited once more followed by points for future work.

11.2 Original contributions

The original contributions achieved in this thesis are listed below:

- In Chapter 3, a generic and domain independent novel frame, KDD-IDSS, was established for integrating knowledge discovery in databases with intelligent decision support systems. It automated the overall decision-making process, beginning with the ability of problem recognition and ending with a continuous feedback about the decision's outcome.

- Chapter 3 also presented a constrained logic programming based meta-language for interfacing optimisation and AI modules in the KDD-IDSS frame. The language represented

a level of abstraction used to isolate the user from the problem solving details. A mate-selection example was used to illustrate the potential usefulness of this language.

- In Chapter 4, the rules governing the outcome of a mating were extracted from the dairy database using RULEX and C5. Autoclass was used to discretise the inputs and the output. The domain expert suggested that discrete inputs are more comprehensible than continuous inputs. Therefore, C5 was chosen since it produced less rules than RULEX with similar accuracy.

- Chapter 5 introduced a novel algorithm, C-Net, for integrating ANNs and DTs. The algorithm achieved a performance which was intermediate to this achieved by neural networks and decision trees in isolation. It outperformed the C5 algorithm in terms of classification error and used a representational language simpler than the neural network from which it was extracted. On some of the datasets, C-Net even generalised better than the neural network from which it was extracted.

- In Chapter 7, a multi-stage mate-selection problem was formulated generically. The complexity of the problem was examined and it was found that solving this problem to optimality is impossible with the current state-of-the-art in optimisation theory. To my knowledge, this is the first time EAP was generically formulated.

- Chapter 8 presented a single-stage mate-selection model, simplified from the generic formulation presented in Chapter 7. The model was formulated as a quadratic transportation model, and genetic algorithm was used to solve it. A repair operator was developed to retrieve the feasibility of the chromosomes. Also, a new crossover operator, called gene-based crossover, was developed. The best GA result was achieved with the one-point crossover operator with modified tournament selection.

- Chapter 9 introduced a multi-stage mate-selection problem for farms dependent on artificial insemination. The model was derived from the generic model and a methodical set of experiments was undertaken to examine a suitable heuristic technique for solving this problem. Random search, sequential genetic algorithms, hill climbing, genetic algorithms, simulated annealing, ant colony optimisation, and immune systems were all examined for solving this model. Additionally, a new heuristic search strategy was developed, called

Markov-chain Tabu search, for solving the problem. Furthermore, a new hybrid-algorithm (ACO+GA) for evolving colonies of ants by combining ant colony optimisation and genetic algorithms was developed. The ACO+GA hybrid resulted in the best performance among the population based algorithms (which included Sequential GA, ACO, GA, and Immune) whereas Markov-chain Tabu search (MCTS) resulted in the best overall performance.

- In Chapter 10, a method for creating a mate-selection index, called *dynamic adjustment of the objective function*, was introduced. The theoretical foundations for this method were established and two hybrid algorithms, simulated annealing-genetic algorithms (SA+GA) hybrid, and differential evolution-genetic algorithms (DE+GA) hybrid, were developed and tested. The latter resulted in the better performance of the two methods.

11.3 Future work

This thesis presented an overall information system framework (KDD-IDSS) for the efficient design of breeding programs. No work is ever truly complete; otherwise we should stop research. Some interesting research questions therefore arise from this work. A list is given below in two categories; information technology points of further research and agriculture ones.

1. Future work from information technology point of view

    - The first research point is how to extend the design of the meta-language to cover all aspects of the KDD-IDSS. The KDD-IDSS has a hierarchal architecture consisting of agents which control other agents and controlled by other agents. This leads us to think of each predicate as an agent which is responsible for a specific task. Each module in the KDD-IDSS is also responsible from an agent which co-ordinates the other agents. Therefore, we have a hierarchal architecture for the KDD-IDSS using multi-agent systems. In this case, the meta-language defines the communication language among the agents and a description for the overall task the agent can do.
    - Building up a prototype of the KDD-IDSS system is a very important open question. It is a multi-disciplinary project that requires a team of scientists. From a practical perspective, the proposed system is achievable, based on my own experience. The expected profit from developing such a system would be very high since the system

will not be developed just for farmers or the mate-selection problem. Because of its modularity, the system can be used for many problems like transportation and budget programming.

- The dynamic decision trees concept, (C-Net, Chapter 5), is a new concept introduced in this thesis and it has lots of potential. For example, using the approach presented in the thesis for integrating artificial neural networks and decision trees, can be a means for extracting and representing finite state automaton from recurrent neural networks. Furthermore, the applications of dynamic decision trees are enormous and this opens a new area of research in this direction.

2. Future work from animal breeding point of view

- Developing more techniques for decomposing and handling the multi-stage model is also an open question. More studies can be undertaken in this area to compare the results obtained in the thesis against new technologies emerging in the future.
- Analysing the underlying dairy principles in the optimisation process from the breeder perspective. It was sufficient for us to show that the total objective value for the multi-stage model is better than that obtained from the sequential GA experiment. But, what is the economic value of this improvement? Moreover, instead of scaling the objectives to overcome the magnitude problem, can we develop an economic model which calculates precisely the economic value of each objective? These are still open questions that need the employment of economic models which can be a very interesting piece of research if undertaken properly.
- Selectabull as discussed in Chapter 2 does not consider the mate-selection problem. It would be interested to extend this package with mate-selection. Also, it does not capture important genetic principles such as inbreeding and it would be more appropriate to incorporate inbreeding (both short and long term) within Selectabull.
- *Industrial Significance*: *Total genetic resource management* (TGRM) (Kinghorn and Shepherd 1999) is a breeding aid program driven by specifying desired outcomes (*eg.* outcomes in genetic gains) (Kinghorn and Shepherd 1999). The program was developed by a group of animal breeders from the University of New England led by Prof.

Brian Kinghorn, Dr. Robert Bank, and Dr. Ross Shepherd. It is currently the state of the art in the field of mate-selection. The approach relies on the use of an evolutionary algorithm (differential evolution) for optimising the mating pairs. TGRM demonstrates the importance of mate-selection. I believe that utilising the results of this thesis would improve the performance of TGRM. I may recall that the differential evolution approach did not work as well as the others. Therefore, it would be interesting to apply Markov Chain Tabu Search within the TGRM package and compare the results with the differential evolution approach.

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Appendix A

The rules generated by C5

```
Rule 14: (cover 124)
     dam_season_of_calve = spring
     dam_milk_volume = low
     sire_abv_milk = above_average
->  class low  [0.929]

Rule 20: (cover 114)
     dam_season_of_calve = spring
     dam_milk_volume = low
     sire_abv_milk = high
->  class low  [0.914]

Rule 1: (cover 5020)
     herd_milk_average = low
->  class low  [0.868]

Rule 21: (cover 2832)
     dam_milk_volume = below_average
->  class low  [0.725]

Rule 11: (cover 79)
     dam_season_of_calve = spring
     herd_milk_average = average
     sire_abv_milk = average
->  class low  [0.667]

Rule 3: (cover 359)
     sire_abv_milk = very_low
->  class low  [0.645]

Rule 4: (cover 2596)
     sire_abv_milk = low
->  class low  [0.605]

Rule 19: (cover 3)
     dam_season_of_calve = summer
     herd_milk_average = average
     sire_abv_milk = high
```

```
->  class low  [0.600]

Rule 22: (cover 836)
     dam_season_of_calve = spring
     dam_milk_volume = average
->  class low  [0.584]

Rule 2: (cover 4201)
     herd_milk_average = below_average
->  class low  [0.571]

Rule 9: (cover 2378)
     sire_abv_milk = below_average
->  class low  [0.509]

Rule 12: (cover 337)
     dam_season_of_calve = winter
     herd_milk_average = average
     sire_abv_milk = above_average
->  class low  [0.507]

Rule 34: (cover 2)
     herd_milk_average = high
     dam_milk_volume = low
     sire_abv_milk = high
->  class average  [0.750]

Rule 35: (cover 2)
     dam_season_of_calve = autumn
     herd_milk_average = high
     dam_milk_volume = below_average
     sire_abv_milk = high
->  class average  [0.750]

Rule 26: (cover 9)
     dam_season_of_calve = autumn
     herd_milk_average = above_average
     dam_milk_volume = above_average
     sire_abv_milk = below_average
->  class average  [0.727]

Rule 10: (cover 6)
     dam_season_of_calve = summer
     herd_milk_average = average
     sire_abv_milk = average
->  class average  [0.625]

Rule 25: (cover 71)
     herd_milk_average = above_average
     dam_milk_volume = average
     sire_abv_milk = below_average
->  class average  [0.603]

Rule 13: (cover 93)
     dam_season_of_calve = autumn
     herd_milk_average = average
```

```
     sire_abv_milk = above_average
->   class average  [0.579]

Rule 37: (cover 311)
     herd_milk_average = high
     dam_milk_volume = average
->   class average  [0.543]

Rule 23: (cover 148)
     herd_milk_average = average
     dam_milk_volume = above_average
     sire_abv_milk = high
->   class average  [0.540]

Rule 17: (cover 47)
     dam_season_of_calve = spring
     herd_milk_average = average
     dam_milk_volume = high
     sire_abv_milk = above_average
->   class average  [0.531]

Rule 32: (cover 272)
     herd_milk_average = high
     sire_abv_milk = below_average
->   class average  [0.529]

Rule 18: (cover 348)
     dam_season_of_calve = winter
     herd_milk_average = average
     sire_abv_milk = high
->   class average  [0.514]

Rule 33: (cover 259)
     herd_milk_average = high
     sire_abv_milk = average
->   class average  [0.510]

Rule 24: (cover 271)
     herd_milk_average = average
     sire_abv_milk = very_high
->   class average  [0.509]

Rule 29: (cover 2)
     dam_season_of_calve = summer
     herd_milk_average = above_average
     dam_milk_volume = above_average
     sire_abv_milk = very_high
->   class high  [0.750]

Rule 40: (cover 4168)
     herd_milk_average = very_high
->   class high  [0.691]

Rule 31: (cover 1285)
     dam_milk_volume = high
     sire_abv_milk = very_high
```

```
->  class high  [0.632]

Rule 39: (cover 278)
     herd_milk_average = high
     sire_abv_milk = very_high
->  class high  [0.575]

Rule 38: (cover 2363)
     dam_milk_volume = high
     sire_abv_milk = high
->  class high  [0.556]

Rule 28: (cover 84)
     dam_season_of_calve = autumn
     herd_milk_average = above_average
     sire_abv_milk = very_high
->  class high  [0.512]
```

Appendix B

The Code for the Markov Chain Tabu Search Algorithm

```
//Title:        Markov Chain Tabu Search
//Version:
//Copyright:    Copyright (c) 1999
//Author:       Hussein Aly Abbass
//Company:      Machine Learning Research Center
//Description:  The main contoller for MCTS

#include <stdlib.h>
#include <math.h>
#include <iostream.h>
#include <fstream.h>
#include <iomanip.h>
#include <string.h>
#include <assert.h>

#include "MCTS_Operator.h"

Operator ee2;
void     GA_read_parameter_file();

main(int argc,char *argv[])
{
 GA_read_parameter_file();
 if (argc != 10)
     {
      cout << endl << endl;
      cout << "There should be 7 parameters                " << endl;
      cout << "--------------------------                  " << endl;
      cout << "00- Seed                                    " << endl;
      cout << "01- Number_of_runs                          " << endl;
      cout << "02- Number_of_children                      " << endl;
      cout << "03- Maximum_number_of_mating_per_sire       " << endl;
      cout << "04- Number_of_generations                   " << endl;
      cout << "05- Neighbourhood_size                      " << endl;
```

```
      cout << "06- Neighbourhood_length                    " << endl;
      cout << "07- Discount step                           " << endl;
      cout << "08- Threshold                               " << endl;
      exit(1);
     }
  ee2.seed                                  = atol(argv[1]);
  ee2.Number_of_runs                        = atoi(argv[2]);
  ee2.Number_of_children                    = atoi(argv[3]);
  ee2.Maximum_number_of_mating_per_sire     = atoi(argv[4]);
  ee2.Number_of_generations                 = atoi(argv[5]);
  ee2.Neighbourhood_size                    = atoi(argv[6]);
  ee2.Neighbourhood_length                  = atoi(argv[7]);
  ee2.discount_step                         = (double) (atoi(argv[8])/1000.0);
  ee2.Threshold                             = (double) (atoi(argv[9])/1000.0);
  ee2.MCTS_controller();
  return(1);
}

void GA_read_parameter_file()
{
 int c;
 char attribute[40];
 ifstream ga_parameter_file("Hussein", ios::in);
 if(!ga_parameter_file) { cerr << "file Hussein not opened" << endl; exit(1); }
 while ((c=ga_parameter_file.get()) != EOF)
 {
  if (c == '#')
  {
   c = ga_parameter_file.get();
   ga_parameter_file >> attribute;
   if (strcmp(attribute,"SIGMA_ABV") == 0)
      ga_parameter_file >> ee2.SIGMA_ABV;
   else if (strcmp(attribute,"Variance_PRICE") == 0)
           ga_parameter_file >> ee2.Variance_PRICE;
   else if (strcmp(attribute,"Phenotypic_PRICE") == 0)
           ga_parameter_file >> ee2.Phenotypic_PRICE;
   else if (strcmp(attribute,"Genotypic_PRICE") == 0)
           ga_parameter_file >> ee2.Genotypic_PRICE;
   else if (strcmp(attribute,"Inbreeding_PRICE") == 0)
           ga_parameter_file >> ee2.Inbreeding_PRICE;
   else if (strcmp(attribute,"Coancestory_PRICE") == 0)
           ga_parameter_file >> ee2.Coancestory_PRICE;
   else if (strcmp(attribute,"Culling_PRICE") == 0)
           ga_parameter_file >> ee2.Culling_PRICE;
   else {cout << "ERROR in the parameter file with attribute "
           << attribute << " IGNORED" << endl;c = ' ';}
  } else {while ((c != '\n') && (c != EOF)) c = ga_parameter_file.get();
           if (c == EOF) ga_parameter_file.putback((char) c);}
 }
 ga_parameter_file.close();
}
```

```
//Title:        Markov Chain Tabu Search
//Version:
//Copyright:    Copyright (c) 1999
//Author:       Hussein Aly Abbass
//Company:      Machine Learning Research Center
//Description:  The random number generator for MCTS

#ifndef _RANDOM_H
#define _RANDOM_H

#include <stdlib.h>
#include <math.h>

class Random {
public:
Random();
double nextDouble();
double nextGaussian();
double nextGaussian(double,double);
void   setSeed(int);
void   setSeed(long);
private:
        long  idum;   // this is the seed
        long    IA;
        long    IM;
        double  AM;
        long    IQ;
        long    IR;
        long    NTAB;
        double  NDIV;
        double  EPS;
        double  RNMX;
        long iy;
        long *iv;
};

Random::Random()
{
 idum = (long) -12345; // this is the seed
 IA   = 16807;
 IM   = 2147483647;
 AM   = (1.0/IM);
 IQ   = 127773;
 IR   = 2836;
 NTAB = 32;
 NDIV = (1.0+(IM-1.0)/(double) NTAB);
 EPS  = 1.2e-7;
 RNMX = (1.0-EPS) /* largest double less than 1 */;
 iy=0;
 iv = new long[NTAB]; assert((iv)!= 0);
}

void Random::setSeed(int X) { idum = (long) -X; }

void Random::setSeed(long X) { idum = -X; }
```

```
double Random::nextGaussian(double mean,double stdev)
{
double x = (double) nextGaussian();
return (double) (x * stdev + mean);
}

double Random::nextDouble()
{
 int j;
 long k;
 double temp;
 if (idum <=0 || !iy)
    {
     if (-idum < 1) idum=1; else idum = -idum;
     for (j=NTAB+7;j>=0;j--)
         {
          k = (long) (idum / (double) IQ );
          idum=IA*(idum-k*IQ)-IR*k; if (idum < 0)
                   idum +=IM; if (j < NTAB) iv[j] = idum;
         }
     iy=iv[0];
    }
 k= (long) (idum/ (double) IQ );
 idum=IA*(idum-k*IQ)-IR*k;
 if (idum < 0) idum += IM;
 j= (int) (iy/NDIV);
 iy=iv[j];
 iv[j]= idum;
 if ((temp=AM*iy) > RNMX) return RNMX; else return temp;
}

double Random::nextGaussian()
{
 static int iset=0;
 static double gset;
 double fac,rsq,v1,v2;
 if (iset ==0)
    {
     do
       {
        v1=2.0*nextDouble()-1.0; v2=2.0*nextDouble()-1.0; rsq=v1*v1+v2*v2;
       }
     while(rsq>=1.0 ||rsq ==0.0);
     fac =sqrt(-2.0*log(rsq)/(double) rsq);
     gset=v1*fac;'
     iset=1;
     return v2*fac;
    }
    else
    {
     iset=0;
     return gset;
    }
}
#endif
```

```
//Title:        Markov Chain Tabu Search
//Version:
//Copyright:    Copyright (c) 1999
//Author:       Hussein Aly Abbass
//Company:      Machine Learning Research Center
//Description:  The objective evaluator for MCTS

#ifndef _OBJECTIVE_H
#define _OBJECTIVE_H

#include <math.h>
#include <assert.h>

#include "MCTS_Random.h"

class Objective {
public:
                        Objective();
        void            Initialise();

        double          Evaluate_individual(int,int **);

        void            Repair_Chromosome(Random &,int **);

        int             number_of_genes;

        int             Number_of_animals_in_previous_generations;
        int             Number_of_available_dams;
        int             Number_of_available_sires;
        int             Number_of_generations;
        int             Maximum_number_of_mating_per_sire;
        int             Number_of_culling;
        int             Number_of_children;

        double          Phenotypic_PRICE;
        double          Genotypic_PRICE;
        double          Inbreeding_PRICE;
        double          Coancestory_PRICE;
        double          Culling_PRICE;
        double          Variance_PRICE;

        double          STDEV_PE;
        double          STDEV_E;
        double          SIGMA_ABV;

        double          T_genotype;
        double          T_phenotype;
        double          T_inbreeding;
        double          T_coancestry;
        double          T_culling;
        double          T_variance;

private:

        int Number_of_animals_in_current_generation;
        int Number_of_animals_in_all_generations;
```

```
        double *F;
        double **A;

        int             *Pedigree_mother;
        int             *Pedigree_father;
        int             *Dam_id;
        double          *Dam_ABV;
        double          *Dam_P;

        int             *Sire_nmat;
        int             *Sire_id;
        double          *Sire_ABV;

        int             *Dam_id_0;
        double          *Dam_ABV_0;
        double          *Dam_P_0;

int             *culled_animals;
int             *mated_animals;
};

Objective::Objective()
{
 ifstream A_file("Pedigree",ios::in);
 if (!A_file){cerr << "file Pedigree is not opened" << endl;exit(1);}
 A_file >> Number_of_animals_in_previous_generations;
 A_file >> Number_of_available_sires;
 A_file >> Number_of_available_dams;
 A_file.close();
}

void Objective::Initialise()
{
 int i,j,f,m,k,Father,Mother,Gender,Availability;
 int koko;

 ifstream A_file("Pedigree",ios::in);
 if (!A_file){cerr << "file Pedigree is not opened" << endl;exit(1);}
 A_file >> i >> i >> i;

 Number_of_animals_in_current_generation   =
    Number_of_children + Number_of_animals_in_previous_generations;
 Number_of_animals_in_all_generations      =
    Number_of_children * Number_of_generations +
    Number_of_animals_in_previous_generations;

 F                 = new double[Number_of_animals_in_all_generations];
    assert(F != 0);
 Pedigree_mother   = new int[Number_of_animals_in_all_generations];
    assert(Pedigree_mother != 0);
 Pedigree_father   = new int[Number_of_animals_in_all_generations];
    assert(Pedigree_father != 0);

 Dam_id            = new int[Number_of_available_dams];
```

```
   assert(Dam_id != 0);
 Dam_ABV           = new double[Number_of_available_dams];
   assert(Dam_ABV != 0);
 Dam_P             = new double[Number_of_available_dams];
   assert(Dam_P != 0);

 Dam_id_0          = new int[Number_of_available_dams];
   assert(Dam_id != 0);
 Dam_ABV_0         = new double[Number_of_available_dams];
   assert(Dam_ABV != 0);
 Dam_P_0           = new double[Number_of_available_dams];
   assert(Dam_P != 0);

 Sire_nmat         = new int[Number_of_available_sires];
   assert(Sire_nmat != 0);
 Sire_id           = new int[Number_of_available_sires];
   assert(Sire_id != 0);
 Sire_ABV          = new double[Number_of_available_sires];
   assert(Sire_ABV != 0);

 culled_animals    = new int[Number_of_children];
   assert(culled_animals != 0);
 mated_animals     = new int[Number_of_children];
   assert(mated_animals != 0);

 A = (double **) new double[Number_of_animals_in_all_generations];
   assert(A != 0);
 for (i=0;i<Number_of_animals_in_all_generations;i++)
 {
      A[i] = (double *) new double[Number_of_animals_in_all_generations];
      assert(A[i]!= 0);
 }

for (i=0;i<Number_of_animals_in_all_generations;i++)
 {
     for (j=0;j<Number_of_animals_in_all_generations;j++) A[i][j] = 0.0;
     F[i] = 0;
 }
 for (i=0,m=0, f=0;i<Number_of_animals_in_previous_generations;i++)
 {
      A_file >> k >> Gender >> Availability >> Father >> Mother;
      Pedigree_mother[i] = Mother;
      Pedigree_father[i] = Father;
      if ((Gender == 0) && (Availability == 1))
      {
          A_file >> Sire_ABV[m];
          Sire_id[m]=i;
          if (m<Number_of_available_sires) m++;
      }
      else if((Gender == 1) && (Availability == 1))
      {
          A_file >> Dam_ABV[f]  >> Dam_P[f];
          Dam_id[f]=i;
          Dam_id_0[f]=Dam_id[f];
          Dam_ABV_0[f]=Dam_ABV[f];
          Dam_P_0[f]=Dam_P[f];
```

```
        f++;
      }
      else if((Gender == 1) && (Availability == 0))
          A_file >> koko >> koko;
      else
          A_file >> koko;


      A[i][i] = 1;
      if ((Father != -1) && (Mother != -1))
      {
          for (j=0;j<i;j++)
          {
               A[i][j] = 0.5 * (A[j][Father] + A[j][Mother]);
               A[j][i] = A[i][j];
          }
          A[i][i] += 0.5 * A[Father][Mother];
      }
      else if ((Father == -1) && (Mother != -1))
             for (j=0;j<i;j++)
             {
                  A[i][j] = 0.5 * A[j][Mother];
                  A[j][i] = A[i][j];
             }
       else if ((Father != -1) && (Mother == -1))
             for (j=0;j<i;j++)
             {
                  A[i][j] = 0.5 * A[j][Father];
                  A[j][i] = A[i][j];
             }
      F[i] = A[i][i] - 1;

 }
 A_file.close();
}

void Objective::Repair_Chromosome(Random &Rand,int **individual)
{
 int i,i2,i3,Value,Flage,N_Culling,N_Mating;

 for (i2=0;i2<Number_of_generations;i2++)
     {
          N_Culling = 0;
          for (i=0;i<Number_of_available_sires;i++) Sire_nmat[i] = 0;
          for (i3=0;i3<number_of_genes;i3++)
          {
               Value = (int) individual[i2][i3];
               if (Value >= 0) Sire_nmat[Value]+=1;
                   else if (Value == -1) N_Culling+=1;
          }

// Satisfying the maximum number of mating per sire constraint

          for (i=0;i<Number_of_available_sires;i++)
              if (Sire_nmat[i] > Maximum_number_of_mating_per_sire)
              {
```

```
                for (i3=0;i3<number_of_genes;i3++)
                    if ((individual[i2][i3] == i) && (Rand.nextDouble() < 0.5))
                    {
                        individual[i2][i3] = -2;
                        Sire_nmat[i]-=1;
                        if (Sire_nmat[i] == Maximum_number_of_mating_per_sire)
                           i3 = number_of_genes;
                    }
                i--;
            }

// Satisfying the number of culling constraint

          while (N_Culling > Number_of_culling)
          {
                 i3 = (int) (number_of_genes * Rand.nextDouble());
                 if (individual[i2][i3] == -1)
                 {
                     individual[i2][i3] = -2;
                     N_Culling--;
                 }
          }

          while (N_Culling < Number_of_culling)
          {
                 i3 = (int) (number_of_genes * Rand.nextDouble());
                 if (individual[i2][i3] != -1)
                 {
                     individual[i2][i3] = -1;
                     N_Culling++;
                 }
          }

// Calculating the number of mating constraint

          N_Mating = 0;
          for (i3=0;i3<number_of_genes;i3++)
          {
               Value = (int) individual[i2][i3];
               if (Value >= 0) N_Mating ++;
          }

// Satisfying the number of mating constraint

         while (N_Mating < Number_of_children)
         {
                i3 = (int) (number_of_genes * Rand.nextDouble());
                if (individual[i2][i3] == -2)
                {
                    Flage=0;
                    while (!Flage)
                    {
                      i = (int) (Number_of_available_sires * Rand.nextDouble());
                      if (Sire_nmat[i] < Maximum_number_of_mating_per_sire)
                      {
                          individual[i2][i3] = i;
```

```
                        N_Mating++;
                        Sire_nmat[i]++;
                        Flage=1;
                    }
                }
            }
 }

        while (N_Mating > Number_of_children)
        {
            i3 = (int) (number_of_genes * Rand.nextDouble());
            if (individual[i2][i3] > -1)
            {
                individual[i2][i3] = -2;
                N_Mating--;
            }
        }
 }
}

double Objective::Evaluate_individual(int coutflage,int **Individual)
{
 int i,j,i3,l,i4,SIRE,DAM,DAM_id,SIRE_id,CHECK,Father,Mother,Value,mated,culled;
 int N_anims_all_prev_gens,N_anims_curr_gen,Generation_ID;

 double Pheno_VALUE,Geno_VALUE,Inbr_VALUE,TMP1,TMP2,Coanc_VALUE,Culling_VALUE,Total;
 double Variance0, V_2, V, Variance_VALUE;

 T_inbreeding = 0;
 T_coancestry = 0;
 T_genotype   = 0;
 T_phenotype  = 0;
 T_culling    = 0;
 T_variance   = 0;

 for (i=0;i<Number_of_available_dams;i++)
     {
      Dam_id[i] = Dam_id_0[i];
      Dam_ABV[i] = Dam_ABV_0[i];
      Dam_P[i] = Dam_P_0[i];
     }
 l = Number_of_animals_in_previous_generations;
 for (Generation_ID=0;Generation_ID<Number_of_generations;Generation_ID++)
 {
   N_anims_all_prev_gens = Number_of_children * Generation_ID +
               Number_of_animals_in_previous_generations;
   N_anims_curr_gen      = Number_of_children * (Generation_ID + 1)
               + Number_of_animals_in_previous_generations;

   // Updating the A matrix
   for (i=0,mated=0,culled=0;i<number_of_genes;i++)
   {
       Value = (int) Individual[Generation_ID][i];
       if (Value == -1) { culled_animals[culled]=i; culled++; }
       if (Value >= 0)
       {
```

```
        mated_animals[mated]=i;
        Pedigree_father[N_anims_all_prev_gens+mated] = Sire_id[Value];
        Pedigree_mother[N_anims_all_prev_gens+mated] = Dam_id[i];
        mated++;
    }
}

for (i=N_anims_all_prev_gens;i<N_anims_curr_gen;i++)
{
    Father = Pedigree_father[i];
    Mother = Pedigree_mother[i];
    A[i][i] = 1;
    for (j=0;j<i;j++) { A[i][j] = 0.5 * (A[j][Father] + A[j][Mother]);
            A[j][i] = A[i][j]; }
    A[i][i] += 0.5 * A[Father][Mother];
    F[i] = A[i][i] - 1;
}

// End of Updating the A matrix
V_2 = 0.0;
V = 0.0;
for (i3=0;i3<number_of_genes;i3++)
{
     Pheno_VALUE   = 0.0;
     Geno_VALUE    = 0.0;
     Inbr_VALUE    = 0.0;
     Coanc_VALUE   = 0.0;
     Culling_VALUE = 0.0;
     CHECK = (int) Individual[Generation_ID][i3];
     if (CHECK > -1)
     {
         SIRE          = CHECK;
         DAM           = i3;
         Geno_VALUE    = (double) (Genotypic_PRICE * 0.5 *
                               (Dam_ABV[DAM]+Sire_ABV[SIRE]));
         V            += Geno_VALUE;
         V_2          += Geno_VALUE * Geno_VALUE;
         Pheno_VALUE   = (double) (Phenotypic_PRICE  * Dam_P[DAM]);
         Inbr_VALUE    = (double) (Inbreeding_PRICE  * F[l]);
         l++;
         TMP1          = 0.0;
         TMP2          = 0.0;
         for (i4=0;i4<number_of_genes;i4++)
             if (Individual[Generation_ID][i4] > -1)
             {
                 SIRE = (int) Individual[Generation_ID][i4];
                 DAM  = (int) i4;
                 SIRE_id = (int) Sire_id[SIRE];
                 DAM_id = (int) Dam_id[DAM];
                 TMP1 += A[i3][SIRE_id];
                 TMP2 += A[i3][DAM_id];
             }
         Coanc_VALUE = (double) (Coancestory_PRICE * (TMP1 + TMP2));
     }
     else if (CHECK == -1) Culling_VALUE = Culling_PRICE;
          else if (CHECK == -2) {DAM = Dam_id[i3]; Inbr_VALUE = (double)
```

```
                                    (Inbreeding_PRICE * F[DAM]);}
        T_inbreeding += Inbr_VALUE;
        T_coancestry += Coanc_VALUE;
        T_culling    += Culling_VALUE;
        T_genotype   += Geno_VALUE;
        T_phenotype  += Pheno_VALUE;
   }
   if (Generation_ID == 0) Variance0 = (double) (V_2 - ( (double)
                                    (V * V / Number_of_children) ) );
      else Variance_VALUE = (double) (V_2 - ( (double)
                                    (V * V / Number_of_children) ) );

   if (Generation_ID != 0)
      if (Variance_VALUE < (0.8 * Variance0)) T_variance += (double)
                (Variance_PRICE * ((Variance0 * 0.8) - Variance_VALUE));

   for (i=0;i<Number_of_children;i++)
   {
       culled = culled_animals[i];
       mated = mated_animals[i];
       Value = (int) Individual[Generation_ID][mated];
       Dam_id[culled] = N_anims_all_prev_gens + i;
       Dam_ABV[culled] = (double) (0.5 * (Dam_ABV[mated]+Sire_ABV[Value]));
       Dam_P[culled] = (double) (5000.0 + 0.5 * (Sire_ABV[Value]+Dam_ABV[mated]));
   }
 }
 T_variance = (double) ( ((int) (T_variance * 1000)) / 1000.0);
 Total         = T_phenotype + T_genotype + T_inbreeding + T_coancestry +
                               T_culling + T_variance;
 if (coutflage == 1) cout << " GT " << setw(8) << T_phenotype << " "
    << setw(8) << T_genotype << " " << setw(8) << T_inbreeding << " "
    << setw(8) << T_coancestry << " " << setw(8) << T_culling << " "
    << setw(8) << T_variance << " " << setw(8) << Total;
 return Total;
}

#endif
```

```
//Title:        Markov Chain Tabu Search
//Version:
//Copyright:    Copyright (c) 1999
//Author:       Hussein Aly Abbass
//Company:      Machine Learning Research Center
//Description:  The operators for MCTS

#ifndef _OPERATOR_H
#define _OPERATOR_H

#include <stdlib.h>
#include <iostream.h>
#include <iomanip.h>
#include <fstream.h>

#include "MCTS_Objective.h"
#include "MCTS_Random.h"

class Operator {
public:

   Operator();

   void     MCTS_controller();
   void     Generate();

   Random   Rand;
   int      number_of_genes;
   long     seed;

   int      Number_of_runs;
   int      Number_of_ants;
   int      Neighbourhood_size;
   int      Neighbourhood_length;

   int      Number_of_available_dams;
   int      Number_of_available_sires;
   int      Number_of_animals_in_previous_generations;
   int      Number_of_children;
   int      Number_of_culling;
   int      Maximum_number_of_mating_per_sire;

   double   discount_step;
   double   Threshold;

   double   Phenotypic_PRICE;
   double   Genotypic_PRICE;
   double   Inbreeding_PRICE;
   double   Coancestory_PRICE;
   double   Culling_PRICE;
   double   Variance_PRICE;

   double   Phenotypic_weight;
   double   Genotypic_weight;
   double   Inbreeding_weight;
   double   Coancestory_weight;
```

```
   double   Culling_weight;
   double   SIGMA_ABV;

   int      Number_of_generations;

private:

   Objective       Obj;

   int BEST;
   int    BEST_IT;

   int    **optimal_solution_vector;
   int    **current_solution_vector;
   int    **new_solution_vector;
   int    *Sire_nmat;

   double  ***Probability;

   double BEST_FITNESS;
   double BEST_INBREEDING;
   double BEST_COANCESTRY;
   double BEST_GENOTYPE;
   double BEST_PHENOTYPE;
   double BEST_CULLING;
   double BEST_VARIANCE;
   double F_optimal;
   double F_0;
   int Iteration;
};

Operator::Operator() {
}

void Operator::MCTS_controller()
{
 int t,i,j,i1,j1,i2,Sire;
 F_optimal = -1.0e99;
 double discount_step = 1.0/Number_of_children;

 Number_of_animals_in_previous_generations = Obj.Number_of_animals_in_previous_generations;
 Number_of_available_dams                  = Obj.Number_of_available_dams;
 Number_of_available_sires                 = Obj.Number_of_available_sires;
 number_of_genes                           = Number_of_available_dams;

 Sire_nmat               = (int *)     new int[Number_of_available_sires];
    assert(Sire_nmat != 0);
 optimal_solution_vector  = (int **)    new int[Number_of_generations];
    assert(optimal_solution_vector != 0);
 current_solution_vector  = (int **)    new int[Number_of_generations];
    assert(current_solution_vector != 0);
 new_solution_vector      = (int **)    new int[Number_of_generations];
    assert(new_solution_vector != 0);

 Probability              = (double ***) new double[Number_of_generations];
    assert(Probability             != 0);
```

```
for (i=0;i<Number_of_generations;i++)
{
    optimal_solution_vector[i] = (int *) new int[number_of_genes];
        assert(optimal_solution_vector[i] != 0);
    current_solution_vector[i] = (int *) new int[number_of_genes];
        assert(current_solution_vector[i]    != 0);
    new_solution_vector[i]     = (int *) new int[number_of_genes];
        assert(new_solution_vector[i]    != 0);
    Probability[i]             = (double **) new double[number_of_genes];
        assert(Probability[i]             != 0);
    for (j=0;j<number_of_genes;j++)
        {
          Probability[i][j]   = (double *) new double[Number_of_available_sires+1];
                    assert(Probability[i][j]   !=0);
          for (i1=0;i1<Number_of_available_sires+1;i1++)
             Probability[i][j][i1] = 1.0/(1.0+Number_of_available_sires);
        }
}


Rand.setSeed(seed);
Obj.Phenotypic_PRICE  = (double) (Phenotypic_PRICE / 160331);
Obj.Genotypic_PRICE   = (double) (Genotypic_PRICE / 14936.3);
Obj.Inbreeding_PRICE  = (double) (Inbreeding_PRICE / 29.6864);
Obj.Coancestory_PRICE = (double) (Coancestory_PRICE / 8152.92);
Obj.Variance_PRICE    = (double) (Variance_PRICE / 641934);
Obj.Culling_PRICE     = Culling_PRICE;

Obj.SIGMA_ABV                                 = SIGMA_ABV;
Obj.number_of_genes                           = number_of_genes;
Obj.Number_of_generations                     = Number_of_generations;

Obj.Maximum_number_of_mating_per_sire         = Maximum_number_of_mating_per_sire;
Obj.Number_of_children                        = Number_of_children;
Obj.Number_of_culling                         = Number_of_children;
Number_of_culling                             = Number_of_children;

Obj.Initialise();

Iteration=0;
cout << "Iteration: " << setw(3) << Iteration;
for (i=0;i<Number_of_generations;i++) for (j=0;j<number_of_genes;j++)
    {
     current_solution_vector[i][j] = -2;
     optimal_solution_vector[i][j] = -2;
    }
int Dam;
for (i=0;i<Number_of_generations;i++)
    {
    j=0;
    while (j<Number_of_culling)
        {
         Dam = (int) (number_of_genes * Rand.nextDouble());
         if ((current_solution_vector[i][Dam] != -1) &&
           (Probability[i][Dam][Number_of_available_sires] > Threshold))
```

```
            {
             current_solution_vector[i][Dam] = -1;
             optimal_solution_vector[i][Dam] = -1;
             j++;
            }
        }
    }

for (i=0;i<Number_of_generations;i++)
    {
     for (j=0;j<Number_of_available_sires;j++) Sire_nmat[j] = 0;
     for (j=0;j<Number_of_children;j++)
         if (current_solution_vector[i][j] != -1)
            while (current_solution_vector[i][j] < 0 )
                  {
                   Sire = (int) (Rand.nextDouble() * Number_of_available_sires);
                   if ((Probability[i][j][Sire] > Threshold) && (Sire_nmat[Sire] <
                        Maximum_number_of_mating_per_sire))
                      {
                       current_solution_vector[i][j] = Sire;
                       optimal_solution_vector[i][j] = Sire;
                       Sire_nmat[Sire] = Sire_nmat[Sire] + 1;
                      }
                  }
    }

F_0 = Obj.Evaluate_individual(1,current_solution_vector);
F_optimal = F_0;
BEST_IT = Iteration;
cout <<  " " << F_optimal << " " << BEST_IT << endl;

t=0;
for (Iteration=1; Iteration<Number_of_runs; Iteration++)
    {
     cout << "Iteration: " << setw(3) << Iteration;
     for (i=0;i<Number_of_generations;i++) for (j=0;j<number_of_genes;j++)
                       current_solution_vector[i][j] = optimal_solution_vector[i][j];
     for (i=0;i<Number_of_generations;i++)
         {
         j = (int) (number_of_genes * Rand.nextDouble());
         for (j1=0;j1<j;j1++)
             {
              Sire = (int) (Rand.nextDouble() * Number_of_available_sires);
              Dam = (int) (number_of_genes * Rand.nextDouble());
              if (Probability[i][Dam][Sire] > Threshold)
                        current_solution_vector[i][Dam] = Sire;
             }
         }
     Obj.Repair_Chromosome(Rand,current_solution_vector);
     F_0 = Obj.Evaluate_individual(1,current_solution_vector);
     cout <<  " " << F_optimal << " " << BEST_IT << endl;
     if (F_0 > F_optimal)
        {
         for (i=0;i<Number_of_generations;i++)
             for (j=0;j<number_of_genes;j++)
                  optimal_solution_vector[i][j] = current_solution_vector[i][j];
```

```
    BEST_IT = Iteration;
    F_optimal = F_0;
   }
Generate();

if (F_0 > F_optimal)
   {
    for (i=0;i<Number_of_generations;i++)
        for (j=0;j<number_of_genes;j++)
            {
             Sire = optimal_solution_vector[i][j];
             if (Sire != -1) Probability[i][j][Sire] -= discount_step;
             else Probability[i][j][Number_of_available_sires] -= discount_step;
             Sire = current_solution_vector[i][j];
             if (Sire != -1) Probability[i][j][Sire] += discount_step;
             else Probability[i][j][Number_of_available_sires] += discount_step;
             optimal_solution_vector[i][j] = Sire;
            }
    BEST_IT = Iteration;
    F_optimal = F_0;
   }
   else
      for (i1=0;i1<Number_of_generations;i1++) for (j1=0;j1<number_of_genes;j1++)
          {
           Sire = current_solution_vector[i1][j1];
           if (Sire != -1) Probability[i1][j1][Sire] -= discount_step;
             else Probability[i1][j1][Number_of_available_sires] -= discount_step;
           Sire = optimal_solution_vector[i1][j1];
           if (Sire != -1) Probability[i1][j1][Sire] += discount_step;
             else Probability[i1][j1][Number_of_available_sires] += discount_step;
          }
t++;
if (t == ((0.091 - Threshold) * 1000))
   {
    t=0;
    for (i1=0;i1<Number_of_generations;i1++)
            {
             for (i=0;i<number_of_genes;i++)
                 {
                  j1   = (int) (number_of_genes * Rand.nextDouble());
                  Sire = (int) (Number_of_available_sires * Rand.nextDouble());
                  while (Probability[i1][j1][Sire] == Threshold)
                        {
                         Probability[i1][j1][Sire] += discount_step;
                         t++;
                        }
                 }
             while (t > 0)
                   {
                    j1   = (int) (number_of_genes * Rand.nextDouble());
                    Sire = (int) (Number_of_available_sires * Rand.nextDouble());
                    if (Probability[i1][j1][Sire] > (Threshold + discount_step))
                       {
                        Probability[i1][j1][Sire] += discount_step;
                        t--;
                       }
```

```
                        }
                    }
                t=0;
               }
          if ((Iteration - BEST_IT) > 3000) Iteration = Number_of_runs+1;
         }

 cout << "Iteration: " << setw(3) << BEST_IT;
 BEST_FITNESS      = Obj.Evaluate_individual(1,optimal_solution_vector);
 cout << " " << F_optimal << " " << BEST_IT << endl;

 BEST_INBREEDING   = Obj.T_inbreeding;
 BEST_COANCESTRY   = Obj.T_coancestry;
 BEST_GENOTYPE     = Obj.T_genotype;
 BEST_PHENOTYPE    = Obj.T_phenotype;
 BEST_CULLING      = Obj.T_culling;
 BEST_VARIANCE     = Obj.T_variance;

// End of Simulated Annealing Algorithm
// ------------------------------------

 cout << "Run Summary                                    " << endl;
 cout << "---------------------------------------------- " << endl;

 cout << "Best_solution_found_at                      : " << BEST_IT << endl;

 cout << "fitness                                     : " << BEST_FITNESS << endl;
 cout << "inbreeding                                  : " << BEST_INBREEDING << endl;
 cout << "coancestry                                  : " << BEST_COANCESTRY << endl;
 cout << "genotype                                    : " << BEST_GENOTYPE << endl;
 cout << "phenotype                                   : " << BEST_PHENOTYPE << endl;
 cout << "culling                                     : " << BEST_CULLING << endl;
 cout << "variance                                    : " << BEST_VARIANCE << endl;

 cout << "seed                                        : " << seed << endl;
 cout << "Number_of_available_dams                    : " << Number_of_available_dams << endl;
 cout << "Number_of_available_sires                   : " << Number_of_available_sires << endl;
 cout << "Number_of_animals_in_previous_generations : " <<
                                        Number_of_animals_in_previous_generations << endl;
 cout << "Number_of_children                          : " << Number_of_children << endl;
 cout << "Number_of_culling                           : " << Number_of_culling << endl;
 cout << "Maximum_number_of_mating_per_sire           : " << Maximum_number_of_mating_per_sire <<
}

void Operator::Generate()
{
 int i,j,jj,k,Sire,Dam;
 int l1,l2,Alloc1,Alloc2,Neighb;
 double F_1;

 for (k=0;k < Neighbourhood_size; k++)
     {
      cout << "Iteration: " << setw(3) << ++Iteration;
      for (i=0;i<Number_of_generations;i++)
          for (j=0;j<number_of_genes;j++)
              new_solution_vector[i][j] = current_solution_vector[i][j];
```

```
    for (i=0;i<Number_of_generations;i++)
        {
         Neighb = (int) (Neighbourhood_length * Rand.nextDouble());
         for (j=0;j < Neighb; j++)
             {
              jj = (int) (Rand.nextDouble() * number_of_genes);
              new_solution_vector[i][jj] = (int)
                   (Rand.nextDouble() * Number_of_available_sires);
             }
        }
    Obj.Repair_Chromosome(Rand,new_solution_vector);
    F_1 = Obj.Evaluate_individual(1,new_solution_vector);
    cout <<  " " << F_optimal << " " << BEST_IT << endl;

    if (F_1 > F_0)
    {
      for (i=0;i<Number_of_generations;i++)
          for (j=0;j<number_of_genes;j++)
              current_solution_vector[i][j] = new_solution_vector[i][j];
      F_0 = F_1;
    }
    if (F_1 > F_optimal)
    {
      for (i=0;i<Number_of_generations;i++)
          for (j=0;j<number_of_genes;j++)
              optimal_solution_vector[i][j] = new_solution_vector[i][j];
      F_optimal = F_1;
      BEST_IT = Iteration;
    }
   }
}

#endif
```